National Aeronautics and Space Administration

HIGH-END COMPUTING CAPABILITY PORTFOLIO

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NASA Advanced Supercomputing Division

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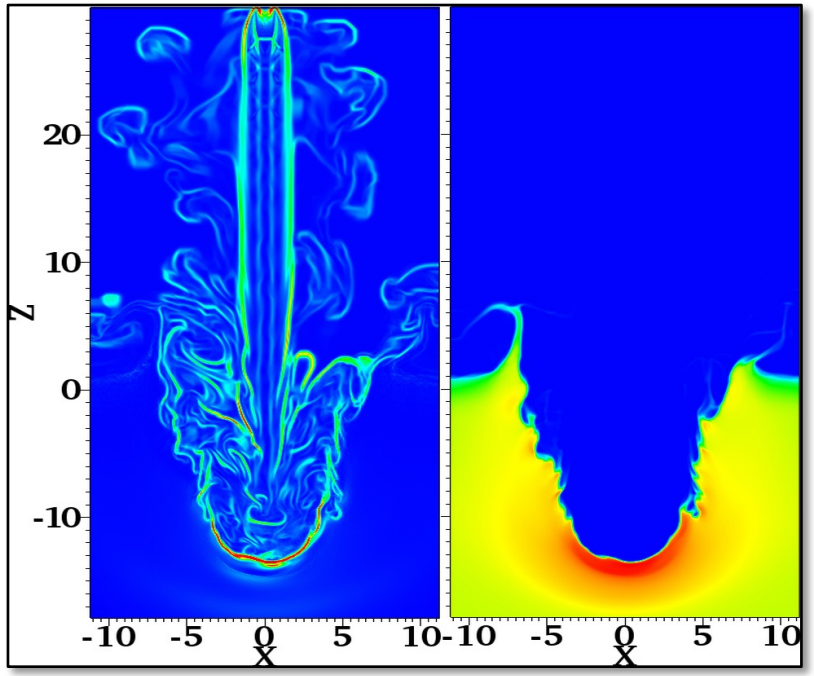
Load Imbalance Monitoring Leads to Significant Improvement for a JPL In-House Application

- HECC's Application Performance and Productivity (APP) team achieved a 2.5x speedup in a Jet Propulsion Laboratory (JPL) in-house parallel application that was identified by system monitoring as needing investigation.
- The JPL in-house code was developed to study the connection between experiments and Large Eddy Simulation model validation for single-phase, two-phase, and supercritical pressure turbulent reactive flows. Validation for a volumetrically dense two-phase flow was done with pressure versus time data from experiments involving a shock interacting with a curtain of solid particles.
- The APP team proactively monitors CPU and memory power usage of all running jobs, looking for load imbalance between the two sockets of any node. The JPL application routinely ran on 16 Rome nodes with 32 MPI ranks per node all running on the first socket, leaving the second socket of all 16 nodes completely idle. By making a simple change to the execution command to include the use of the HECC in-house mbind.x tool to equally spread the processes between the two sockets and pin the processes to CPUs, a 2.5x speedup in each iteration was reported by the user.
- The user has since applied this modification to all their new jobs, which reduces SBU consumption and job turnaround.

IMPACT: Ongoing monitoring of resources such as CPU and memory power usage enables HECC to improve both user turnaround time and overall system utilization.



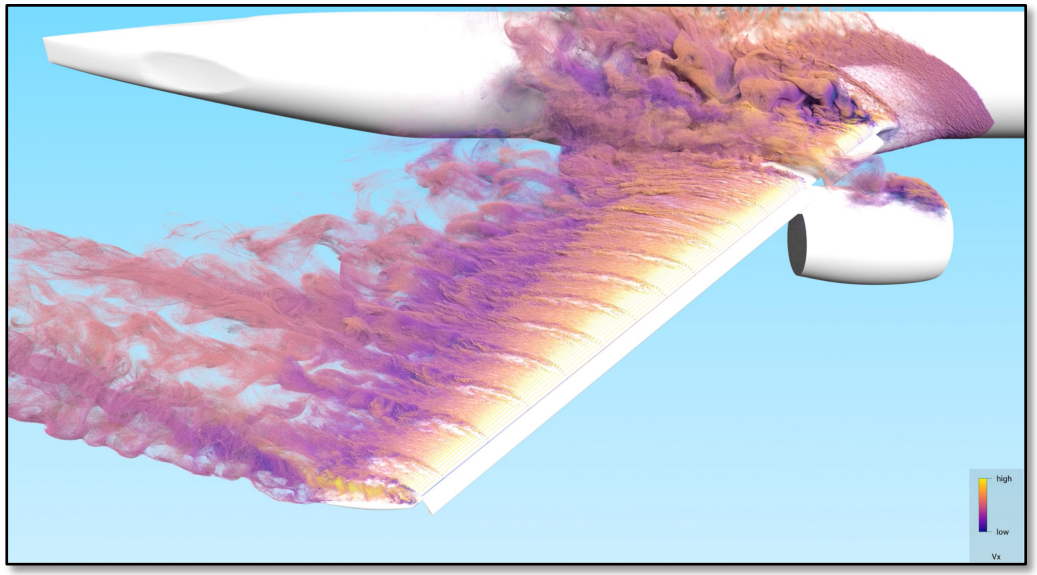
Previous utilization of a large eddy simulation of a turbulent supersonic flow, as represented by the gradient of the true gas density (left) creating a crater in a collection of dense particles as identified by the volume fraction (right). *Kaushik Balakrishnan and Josette Bellan, Jet Propulsion Laboratory*

HECC Supercomputer Usage Sets New Normalized Record

- In March 2023, the combined usage of HECC supercomputers set a new normalized record of 14,046,689 Standard Billing Units (SBUs*).
- The usage by 374 of NASA's science and engineering groups exceeded the previous record of 13,655,190 SBUs set in June 2022 by 391,499 SBUs.
- The record was achieved in great part by the Aeronautics Research Mission Directorate working towards the American Institute of Aeronautics and Astronautics (AIAA) submission deadline.
- Usage of Aitken, Pleaides, Electra, and Endeavour contributed to this record. The new record is greatly attributed to the Aitken Rome nodes, with 128 cores per node.
- The top 10 projects' usage ranged between 182,924 and 2,913,115 SBUs and together accounted for over 52% of the total usage.
- The HECC Project continues to evaluate and plan resources to address the future requirements of NASA's users.

** 1 SBU represents the work that can be done in 1 hour on a Pleiades Broadwell 28-core node.*

IMPACT: The increased capacity of HECC systems and working with users to optimize their run capacities provide mission directorates with more resources to accomplish their goals and objectives.



Particle traces illustrating the flow topology on the suction side of the wing at an angle of attack of 21.5 degrees. The particle trajectories on the outboard part of the wing show the role of slat brackets/ attachments at inducing separation on the outboard section, whereas strong corner flow separation is observed near the wing-body juncture. Particles are colored by their x-component velocity.
Timothy Sandstrom, Gerrit Stich, NASA/Ames

Archive Helper Script Increases Efficiency, Reduces Errors

- HECC Control Room Analysts (CRAs) developed a script that dramatically decreases the effort and time needed to process data archives, reduces the risk of human error when handling data, and improves accuracy with built-in sanity checking. The script more efficiently archives data by automating many of the processes and utilizing built-in templates for communication.
- The script determines which directories the users' data are located in, the amount of data, the project ID (GID) and principle investigator (PI), and if the PI is active; and generates a template to notify PIs of data remaining in the directories for users who are no longer active. The script reduced these steps from ~20 minutes to less than one minute.
  - Previously, multiple options were available at each step after the PI response, which complicated manual processes such as moving between /nobackup filesystems or Lou, or changing ownership. The script generates all the necessary commands to run based on what the PI decides, further reducing the process time and eliminating the risk of human error.
  - Previously, after data transfers were completed, updates to permissions and notifications to users were done manually. Many transfers take an extended amount of time (up to six months), so it took time to remember where the archive files were, confirm them, and write a README file in the retired user's Lou directory.
- The script also allows for simultaneous archiving.

IMPACT: Automation of the data archive process reduced a multi-step manual process from more than an hour down to five minutes, with fewer chances of error, better edge-case troubleshooting and/or documentation, and faster training for staff.

The Lustre tape storage filesystems at the NASA Advanced Supercomputing facility. *NASA Ames*

Physical Installation of Cabeus GPGPU System Completed

- The new General Purpose Graphics Processing Unit (GPGPU) cluster, named Cabeus, will be made available to users as a new 128-node system containing 512 NVIDIA A-100 GPUs and 128 AMD Rome CPUs, adding 5 petaflops of performance to HECC's supercomputing capability.
- HPE completed the final assembly and testing for Cabeus.
  - This includes connections to the InfiniBand fabric, Lustre routers, compute nodes and administrative network.
  - The system will be placed into production in Fall 2023, following significant configuration work, including InfiniBand, front ends, access to shared filesystems, and testing.
- Cabeus will provide a less expensive cost per SBU* on important NASA applications and will further enable NASA work in the artificial intelligence/machine learning space.
- Another 57 NVIDIA V100 GPU nodes and two Nvidia A100 GPU nodes will be added to Cabeus from the Pleiades supercomputer at the end of 2023.

IMPACT: The Cabeus cluster provides a significant increase in graphics processing unit capacity and computational performance to support research engineers and scientists for NASA mission projects.

The new Cabeus supercomputer cluster adds 15 racks and 128 nodes to the main floor of the NASA Advanced Supercomputing facility. *Don Story, NASA Ames*

** 1 SBU equals 1 hour of a Pleiades Broadwell 28-core node.*

ESS Team Completes MacOS Monterey Rollout

- HECC's Engineering Systems and Services (ESS) infrastructure team migrated the fleet of ~220 MacBooks used by staff at the NAS facility to MacOS Monterey.
  - The update is required to enable further security updates.
  - Systems that were unable to run Monterey were excessed. New systems were ordered to replace those outdated laptops.
- The ESS team began the rollout in February 2023, after NASA IT Security approved the Monterey build. These laptop systems are now fully compliant with MacOS requirements.
- Deployment tasks included:
  - Developed a custom build process to address recent Apple hardware restrictions that prevent standard imaging practices.
  - Automated the implementation of NASA IT security benchmarks.
  - Integrated smartcard support with Centrify initially; and later, changed to Apple native Personal Identity Verification (PIV).
- Work has already begun to prepare for the next MacOS upgrade, Ventura, which is expected to begin later in 2023.

IMPACT: HECC's deployment of MacOS Monterey ensures compliance with security mandates that sunset old versions and help protect government data and assets; and enables users to take advantage of the latest Apple software and hardware features.

Screenshot of the Mac OS Monterey splash screen.

APP Team Mentors 2023 Winter Classic Invitational Student Cluster Competition

- HECC's Application Performance and Productivity (APP) team hosted the NASA Module of the student cluster competition organized by Intersect360 Research to provide hands-on HPC experience to 59 students from 12 teams, mostly from Historically Black Colleges and Universities (HBCUs) and Hispanic Serving Institutes (HSIs).
- To streamline the login process, the event utilized 12 clusters set up with the Amazon Web Services (AWS) ParallelCluster tool by the HECC Cloud team. A total of 678 jobs were submitted by the students.
- The APP team selected the opensource Weather Research and Forecasting (WRF) model for the competition and invented a six-component scheme; prepared an online training video and slides; provided guidance via a Meet-and-Greet session, Slack channel discussions, and multiple one-on-one Teams meetings with students who needed extra help.
- The scheme allowed students to work on porting, running, and profiling a real-world application to a new platform. A quiz was devised to test students' understanding and their abilities and interests in scientific research.
- Comments from organizer Dan Olds: "the way you mentored WRF is a great example of how to take inexperienced students through a truly real-like and complex application. I'm going to use it as a model for educating future mentors on how to best take the students through a competition module."
- The NASA Module Results were announced publicly by Intersect360.

IMPACT: The cluster competition—done in multiple modules with Oak Ridge National Laboratory, HPE, and Amazon—empowers students with skills needed in high-performance computing, and gives NASA the opportunity to attract new talent.

Scoring Metrics

Task	Description	Max points	Possible Points	Submission Deadline (PDT)
1	Build netCDF C library	10	0 or 10	Thursday 8 PM
2	Build netCDF Fortran library	10	0 or 10	Thursday 8 PM
3	Build WRF	20	0 or 20	Friday 8 PM
4	Run em_tropical_cyclone case for best price performance	30	between 0 and 30	Sat 8 PM
5	Profile one run with gprof	20	0, 10, 20 or between 10 and 20	Sat 8 PM
6	Answer questions in quiz	10	0, 1 or partial of 1 per question	Sat 8 PM

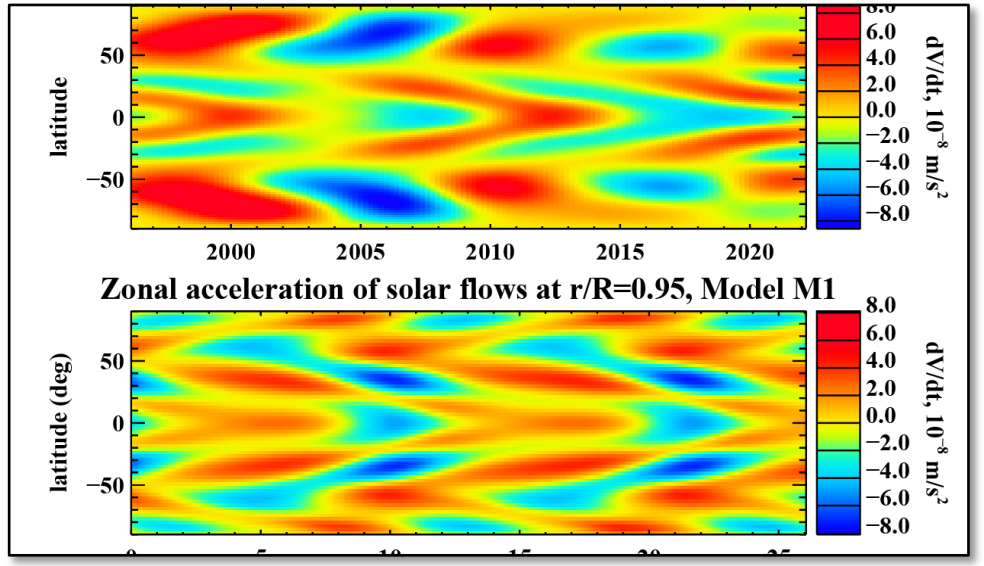
One of the slides included in the cluster competition training materials, depicting the six assigned tasks, the maximum and possible points to be earned, and the corresponding submission deadline. *Sherry Chang, NASA/Ames*

New Findings in Solar Torsional Oscillations and Their Relation to Activity Cycles

- To improve our understanding of how the Sun's magnetic fields generate through a dynamo mechanism, transport to the surface, and form solar activity cycles, physicists at New Jersey Institute of Technology (NJIT) performed computational flow analysis of solar data obtained from two NASA missions in 1996 and 2022, for two sunspot cycles. About 300 terabytes of data were analyzed.
- New results from the data analysis and numerical simulations reveal:
  - Strong evidence of dynamo waves and their migration pattern in the form of two branches migrating toward the poles and the equator, forming an "extended" 22-year solar cycle.
  - Zones of slowdown of the torsional oscillations inside the Sun, caused by magnetic fields generated by the solar dynamo, originating about 120,000 miles beneath the solar surface in a high-latitude region.
  - The zonal flows migrate through the convection zone, revealing patterns of hydromagnetic dynamo waves.
- The numerical simulations reproduce and explain the "extended solar cycle." They confirm the existence of the dynamo waves inside the Sun and provide a basis for developing new capabilities for long-tern predictions of solar activity.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: Enabled by HECC resources, the results from this analysis increase the scientific return from NASA observational missions, and provide a new tool for advanced space weather forecasting.



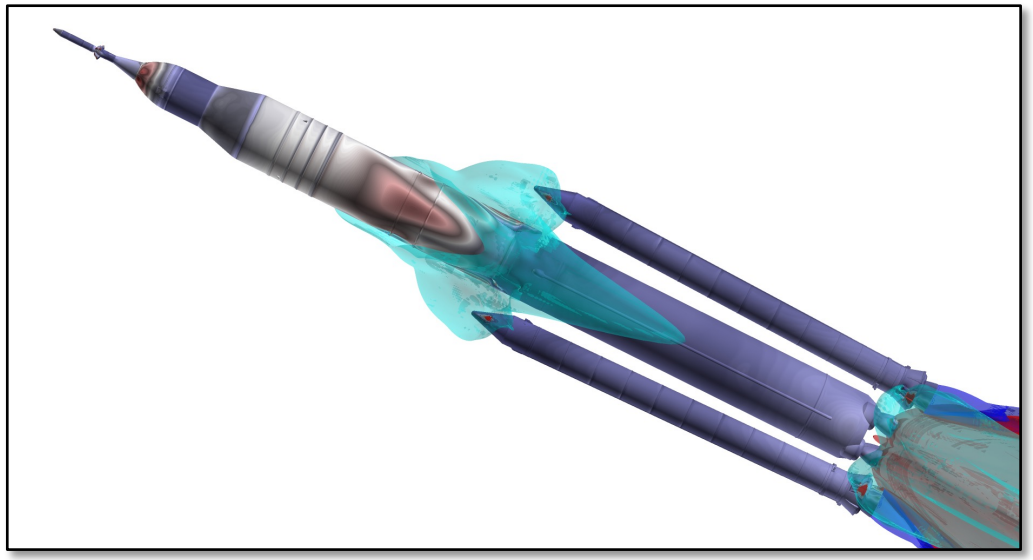
Top: The migrating zonal flows (stream jets) 20,000 miles below the solar surface inferred from helioseismology data from two NASA missions: the Solar and Heliospheric Observatory and Solar Dynamics Observatory. Bottom: The corresponding results of numerical simulations helps to understand the processes of magnetic field generation and the origin of solar magnetic cycles. *Alexander Kosovichev, NJIT*

Building Space Launch System Aerodynamic Databases

- NASA's Artemis program is the agency's mission to return to the Moon by 2025, with the goal to eventually reach Mars. The Space Launch System (SLS) is one the most powerful rockets ever constructed, and it is critical to understand the aerodynamic forces on the rocket and Orion crew vehicle during launch and ascent through Earth's atmosphere. A team of computational fluid dynamics (CFD) researchers in the NASA Advanced Supercomputing Division is developing detailed aerodynamic databases to ensure the safety of the payload and crew.
- The team used CFD simulations with various NASA-developed solvers —including OVERFLOW, FUN3D, and Cart3D—to construct these databases for the ascent and booster separation portions of an SLS launch. Tens of thousands of individual simulations were run supporting various configurations and mission parameters.
- All of the CFD simulations needed to build the databases were run on the Pleiades, Electra, and Aitken supercomputers, with millions of processor hours needed to generate enough data to provide adequate coverage for each simulated phase of flight. It would be impossible to reproduce the data generated for these databases without significant computing resources.

** HECC provided supercomputing resources and services in support of this work.*

IMPACT: These databases are being used by NASA and agency partners across the SLS program and have been utilized for the development of ascent trajectories and for verifying structural integrity. They help ensure the success of all Artemis missions and any future SLS missions.



Isometric view of the Block 1B Space Launch System vehicle simulated during booster separation, showing complex rocket plume interactions where the boosters are eight feet downstream of their attached positions. Vehicle surface is colored by surface pressure (light for low, dark for high). Plumes are illustrated by single color based on origin. *Guy Schauerhamer, Jamie Meeroff, NASA/Ames*

Papers

- "**Shock Heating of Incident Thermal and Superthermal Populations of Different Ion Species**," M. Gedalin, et al., The Astrophysical Journal, vol. 945, no. 1, March 7, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-4357/acb13a/meta
- "**Three-Dimensional Magnetic Reconnection Spreading in Current Sheets of Non-Uniform Thickness,**" M. Arencibia, et al., Journal of Geophysical Research: Space Physics, vol. 128, issue 3, March 9, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2022JA030999
- "**Cavity Ring-Down Spectroscopy of Anthracene, 9-Methylanthreacene, and 2-Methlyanthracene in Supersonic Expansion**," S. Bejaoui, et al., Journal of Physical Chemistry A, vol. 127, issue 12, March 9, 2023. *
  https://pubs.acs.org/doi/abs/10.1021/acs.jpca.2c08994
- "**An Unlikely Survivor: A Low-Density Hot Neptune Orbiting a Red Giant Star**," S. Grunblatt, et al., arXiv:2303.06728 [astro-ph-EP], March 12, 2023. *
  https://arxiv.org/abs/2303.06728
- "**TOI-1695 b: A Water World Orbiting an Early M-Dwarf in the Planet Radius Valley**," C. Cherubim, et al., The Astronomical Journal, vol. 165, no. 4, March 20, 2023. *
  https://iopscience.iop.org/article/10.3847/1538-3881/acbdfd/meta
- "**HD 42477: Coupled r Modes, g Modes, and a p Mode in an AoVnne Star**," D. Kurtz, et al., Monthly Notices of the Royal Astronomical Society, vol. 521, issue 3, March 21, 2023. *
  https://academic.oup.com/mnras/article-abstract/doi/10.1093/mnras/stad858/7083149

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**Conditions for Clump Survival in High-z Disk Galaxies**," A. Dekel, et al., Monthly Notices of the Royal Astronomical Society, vol. 521, issue 3, published online March 21, 2023. *
  https://academic.oup.com/mnras/article-abstract/521/3/4299/7083158?redirectedFrom=PDF
- "**A Helium-Burning White Dwarf Binary as a Supersoft X-ray Source**," J. Greiner, et al., Nature, vol. 615, March 22, 2023. *
  https://www.nature.com/articles/s41586-023-05714-4
- "**Modal Instabilities over Blunted Cones at Angle of Attack in Hypersonic Flow**," P. Paredes, et al., Journal of Spacecraft: Rockets, published online March 23, 2023. *
  https://arc.aiaa.org/doi/full/10.2514/1.A35590
- "**Future Increases in North American Extreme Precipitation in CMIP6 Downscaled with LOCA**," D. Pierce, et al., Journal of Hydrometeorology, published online March 23, 2023. *
  https://journals.ametsoc.org/view/journals/hydr/aop/JHM-D-22-0194.1/JHM-D-22-0194.1.xml
- "**Hydrodynamic Simulations of a Relativistic Jet Interacting with the Intracluster Medium: Application to Cygnus A**," J. ZuHone, et al., Galaxies, vol. 11, issue 2, published online March 23, 2023. *
  https://www.mdpi.com/2075-4434/11/2/51
- "**A High-Eccentricity Warm Jupiter Orbiting TOI-4127**," A. Gupta, et al., arXiv:2303.14570 [astro-ph.EP], March 25, 2023. *
  https://arxiv.org/abs/2303.14570

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Papers (cont.)

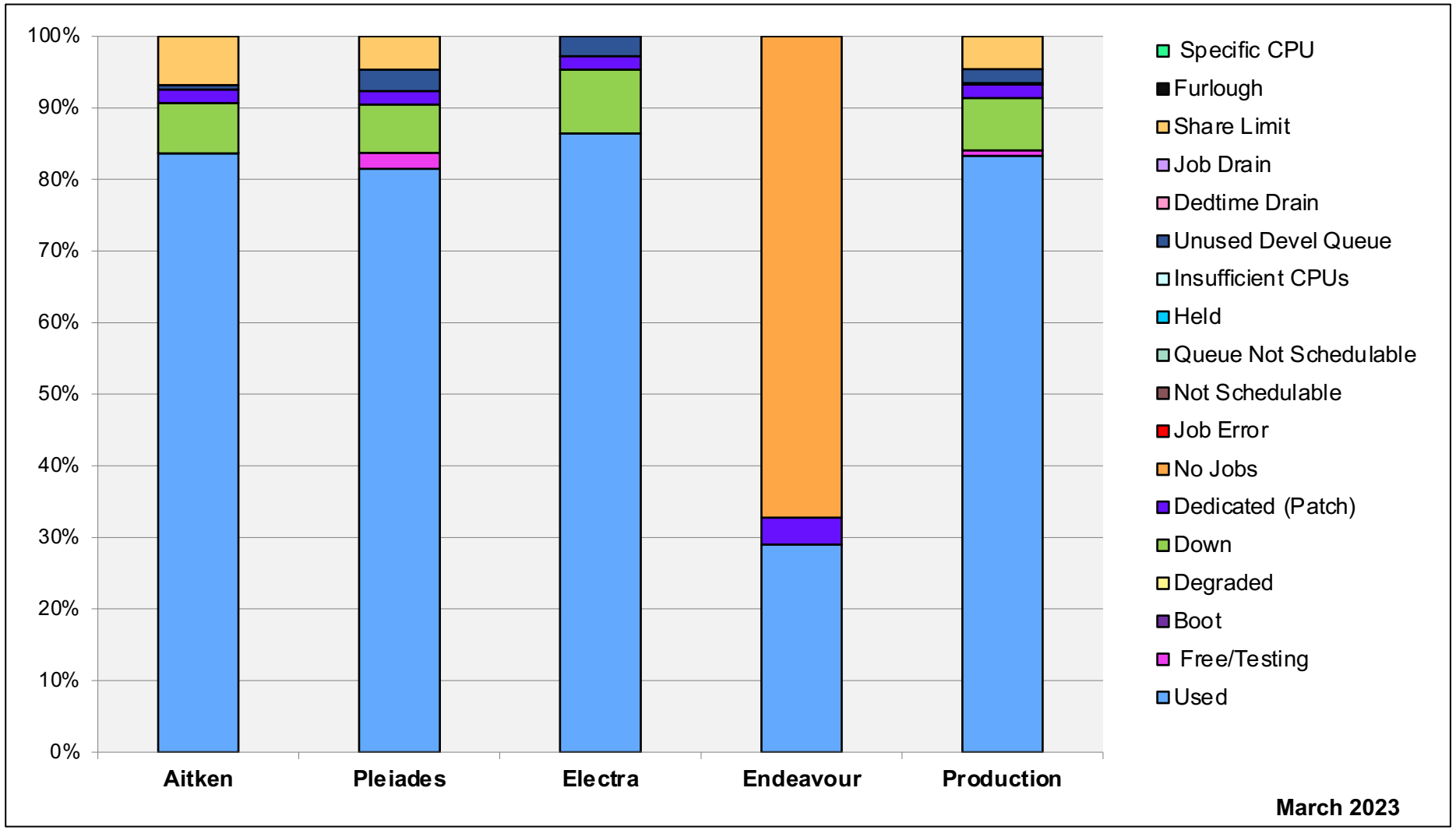
- "**Dynamical Masses of Two Young Transiting Sub-Neptunes Orbiting HD 63433**," M. Mallorquin, et al., arXiv:2303.15411 [astro-ph.EP], March 27, 2023. *
  https://arxiv.org/abs/2303.15411
- "**5-Species MHD Study of Martian Proton Loss and Source**," W. Sun, et al., Journal of Geophysical Research: Space Physics, published online March 28, 2023. *
  https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2023JA031301
- "**Early Bombardment of the Moon: Connecting the Lunar Crater Record to the Terrestrial Planet Formation**," D. Nesvorny, et al., Icarus, published online March 29, 2023. *
  https://www.sciencedirect.com/science/article/abs/pii/S0019103523001227

** HECC provided supercomputing resources and services in support of this work*

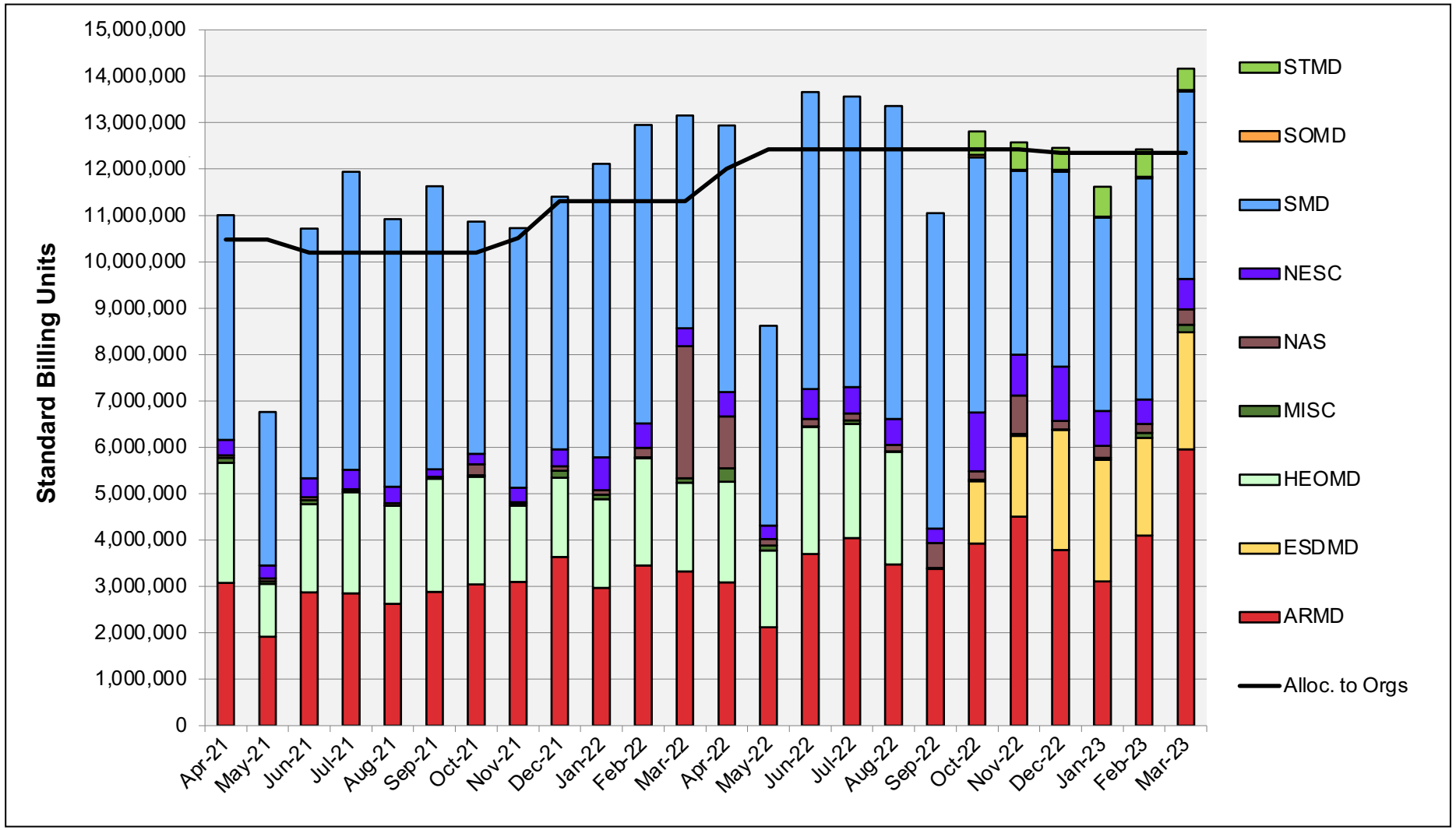
News and Events

- **A Future Aircraft Design, Supercomputed**, *NASA Ames*, March 9, 2023—Ames Research Center features a visualization of turbulence across the Transonic Truss-Braced Wing aircraft concept by the Launch, Ascent, and Vehicle Aerodynamics (LAVA) team performed on the supercomputers at the NASA Advanced Supercomputing facility. *https://www.nasa.gov/aeroresearch/a-future-aircraft-design-supercomputed*
- **Europa's Ice Rotates at a Different Speed from its Interior. Now We May Know Why**, *Universe Today*, March 28, 2023—An international team of researchers hope to answer many questions about the behavior of Europa's interior oceans, in a newly published study, which utilized circulation models run on HECC systems. *https://www.universetoday.com/160740/europas-ice-rotates-at-a-different-speed-from-its-interior-now-we-may-know-why/*

HECC Utilization



HECC Utilization Normalized to 30-Day Month



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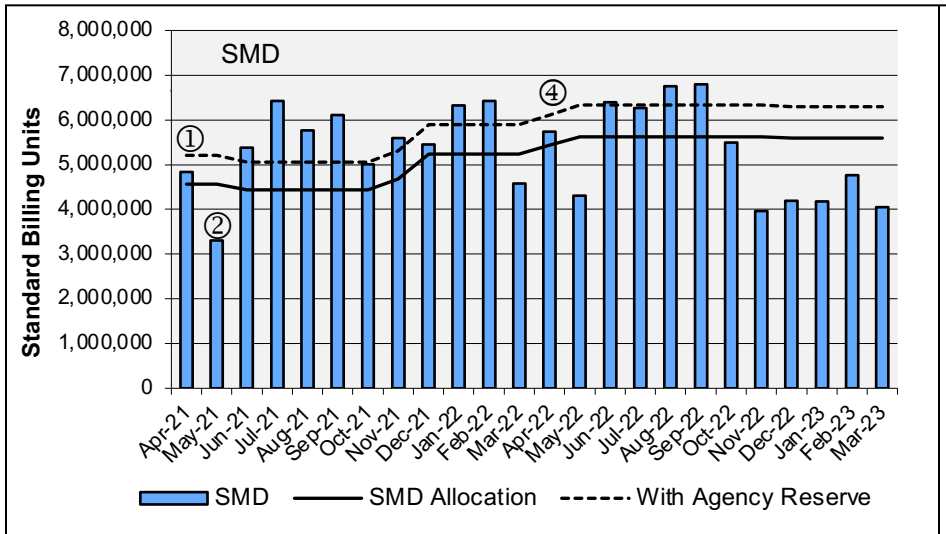
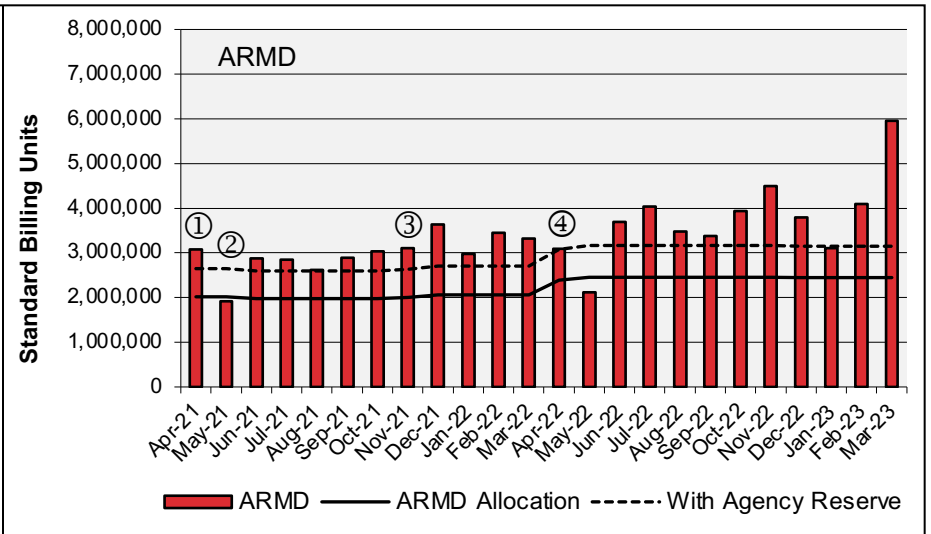
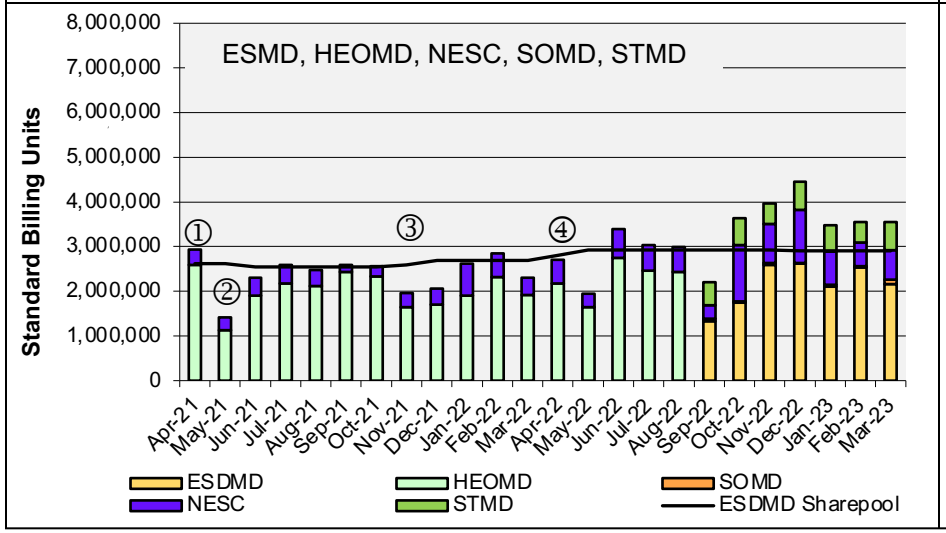






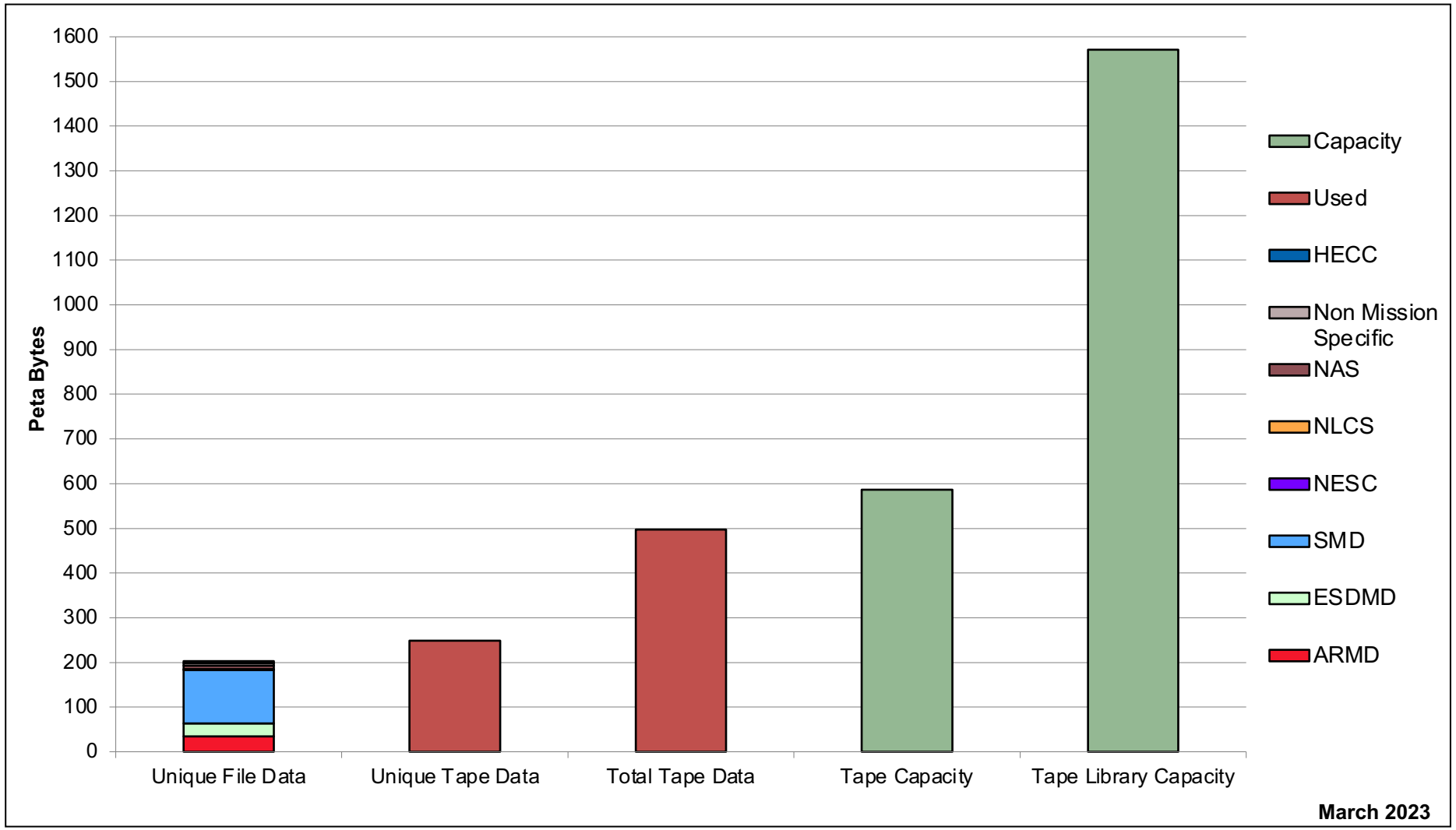
① Endeavour replaced with new hardware

② Merope retired; Annual Maintenance

③ 4 Rome Apollo Racks added to Aitken

④ 4 Rome Apollo Racks added to Aitken

Tape Archive Status



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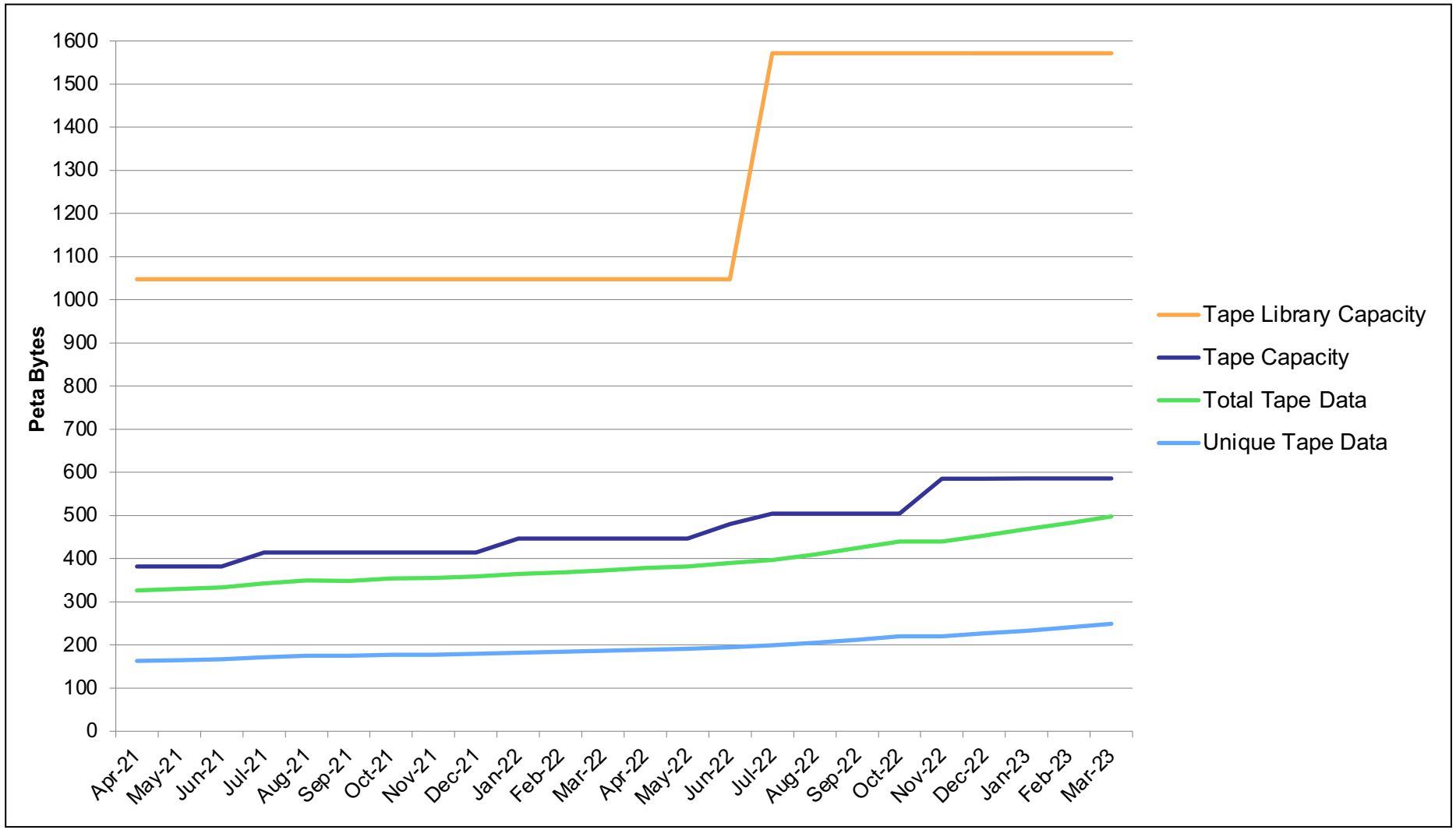
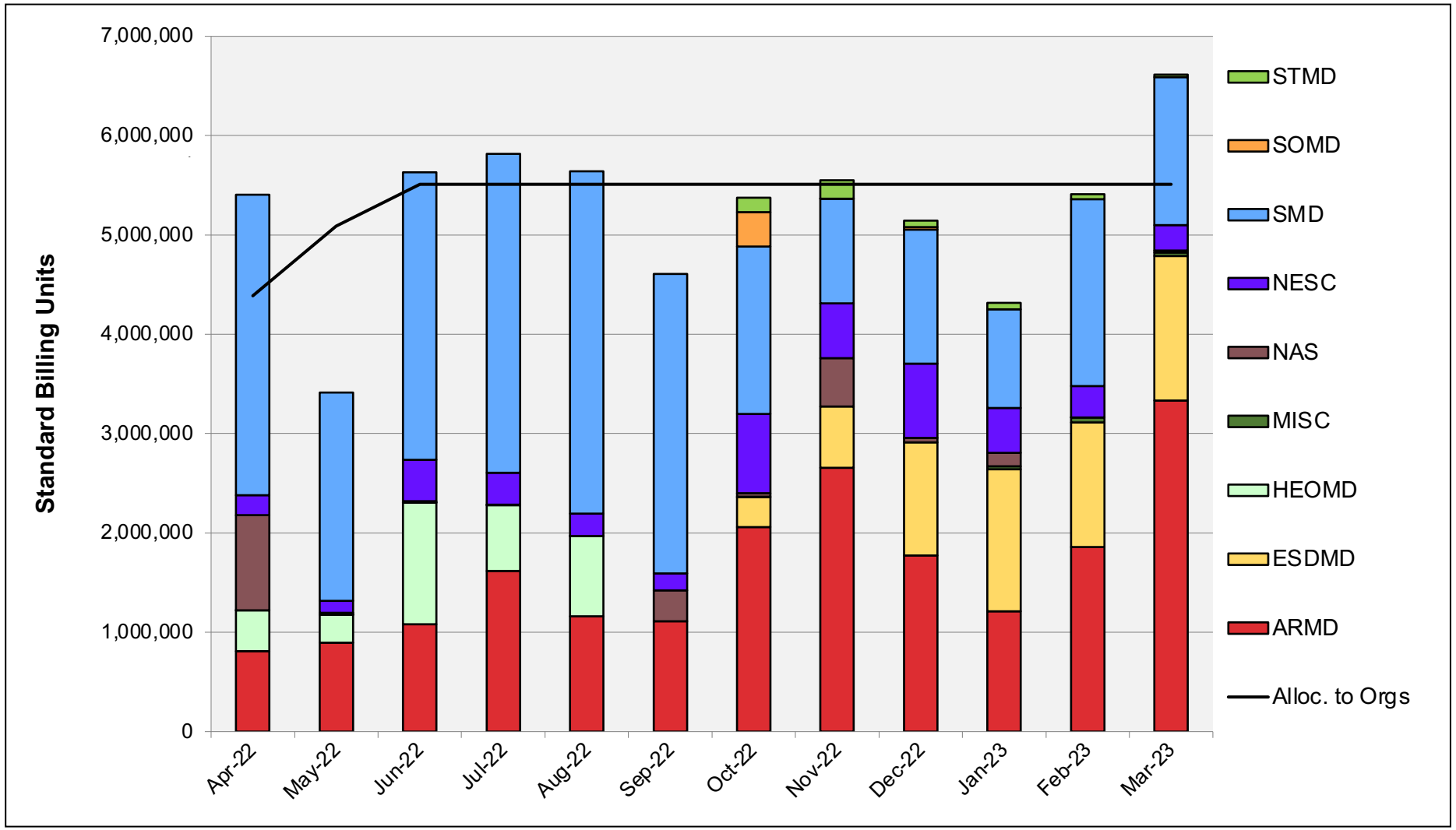
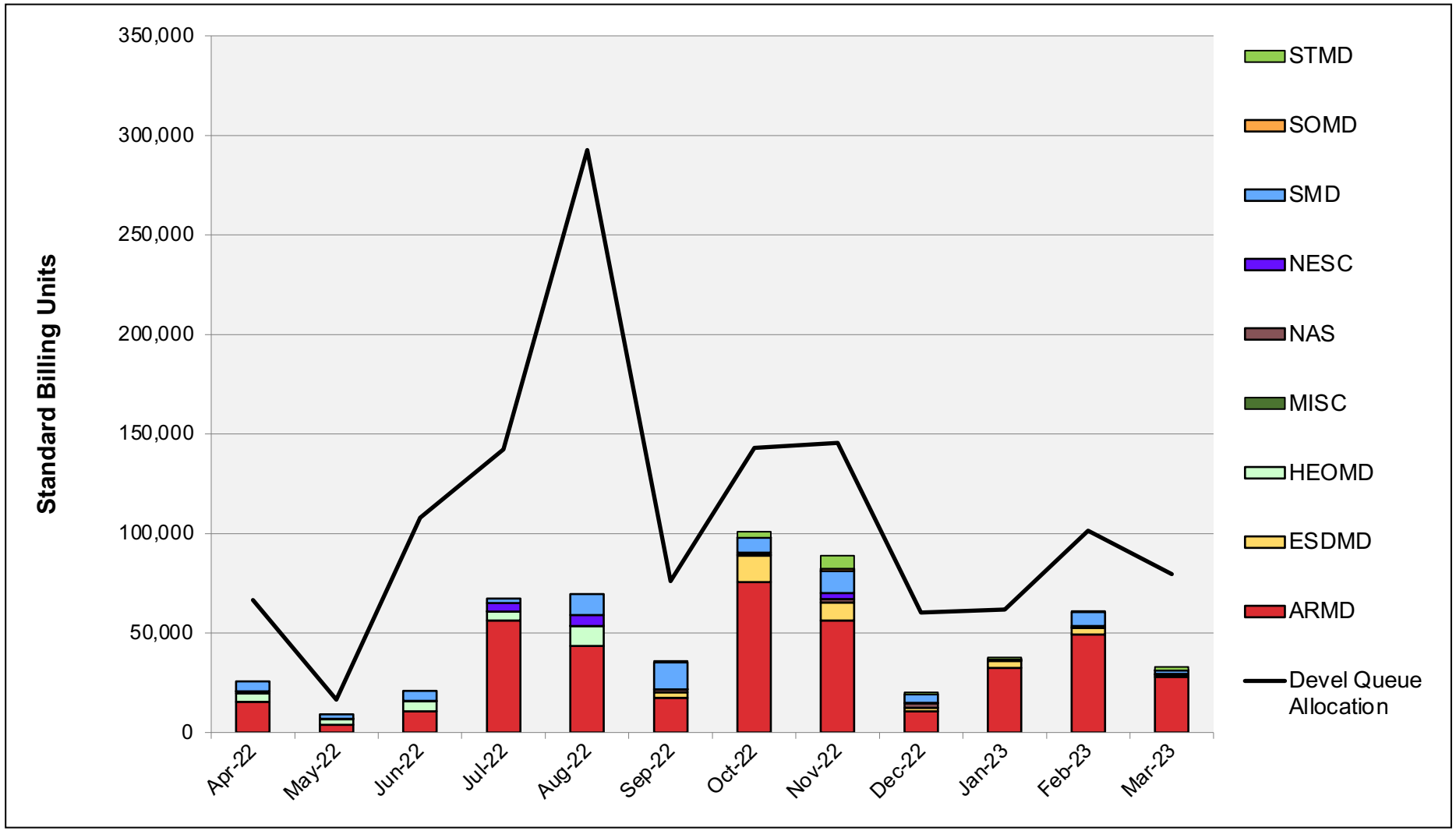


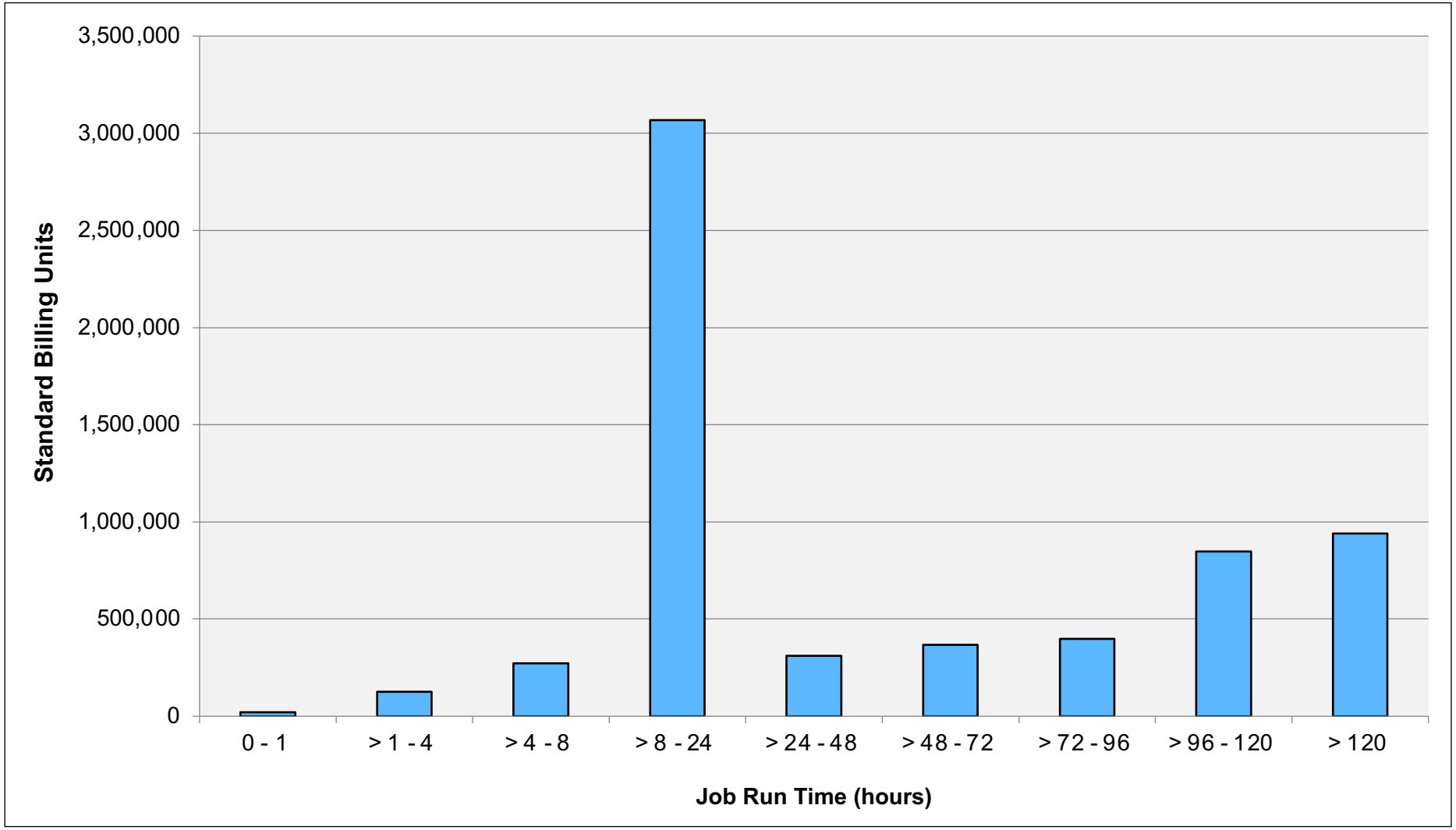
Aitken: SBUs Reported, Normalized to 30-Day Month



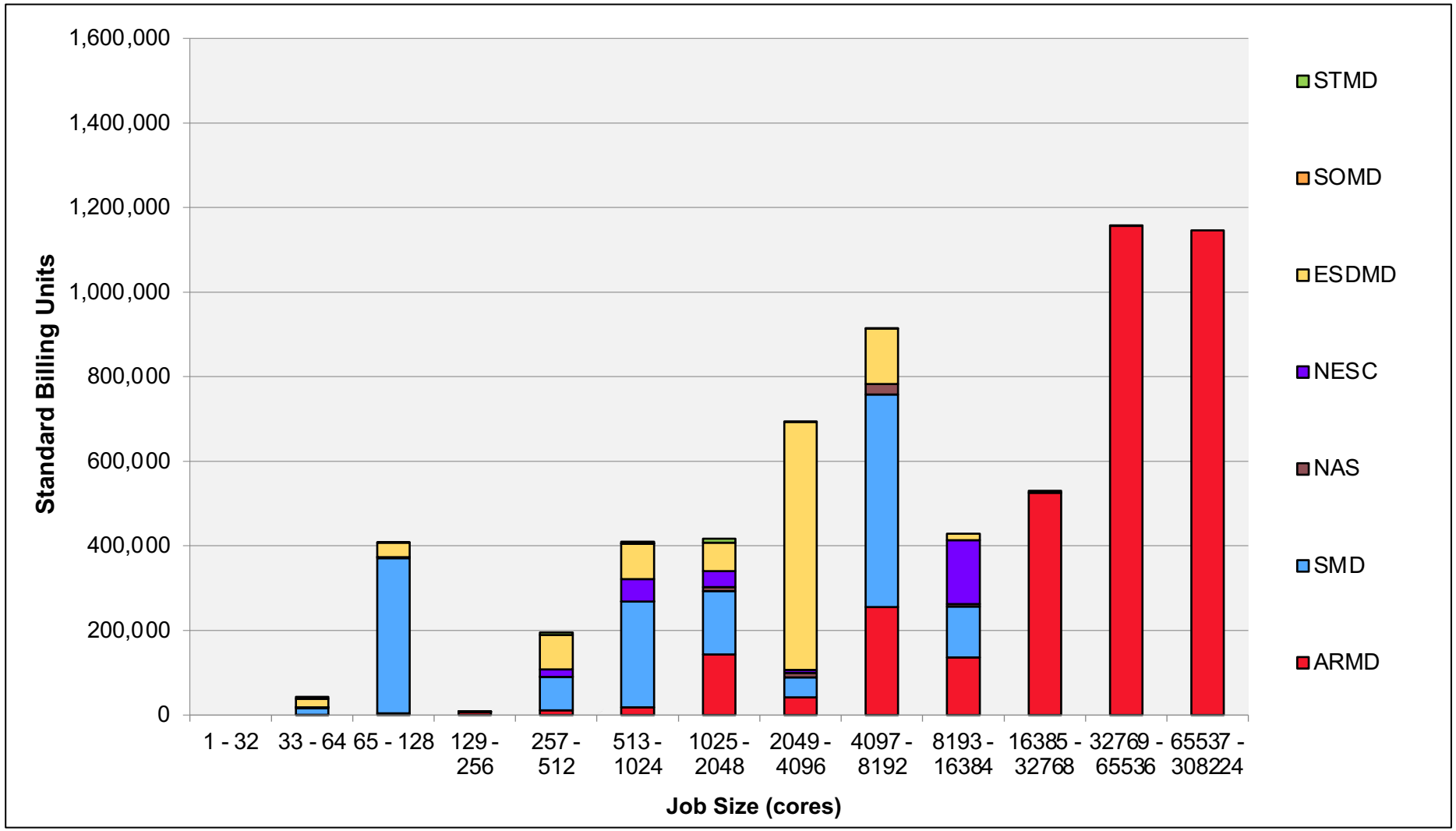
Aitken: Devel Queue Utilization



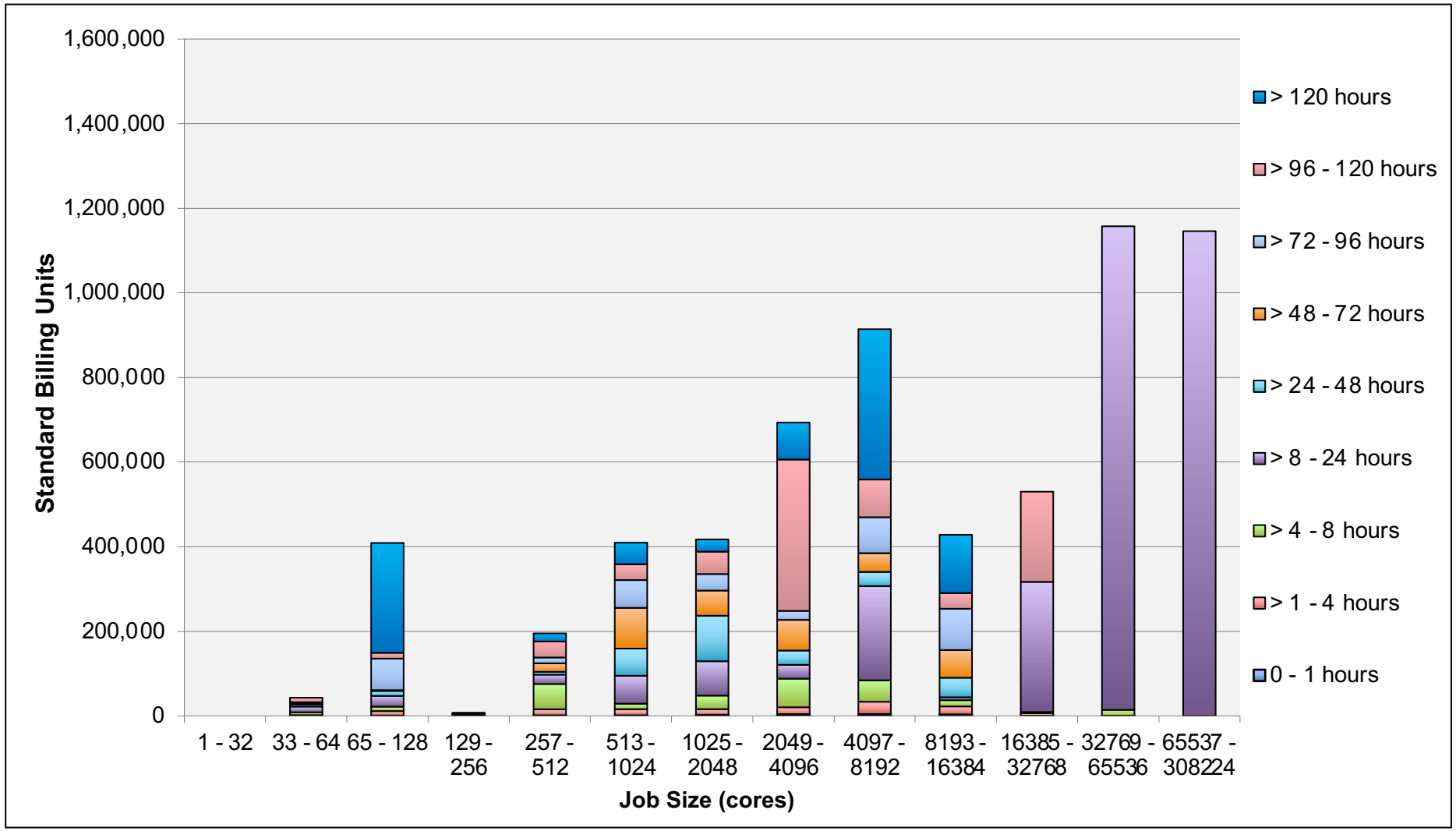
Aitken: Monthly Utilization by Job Length



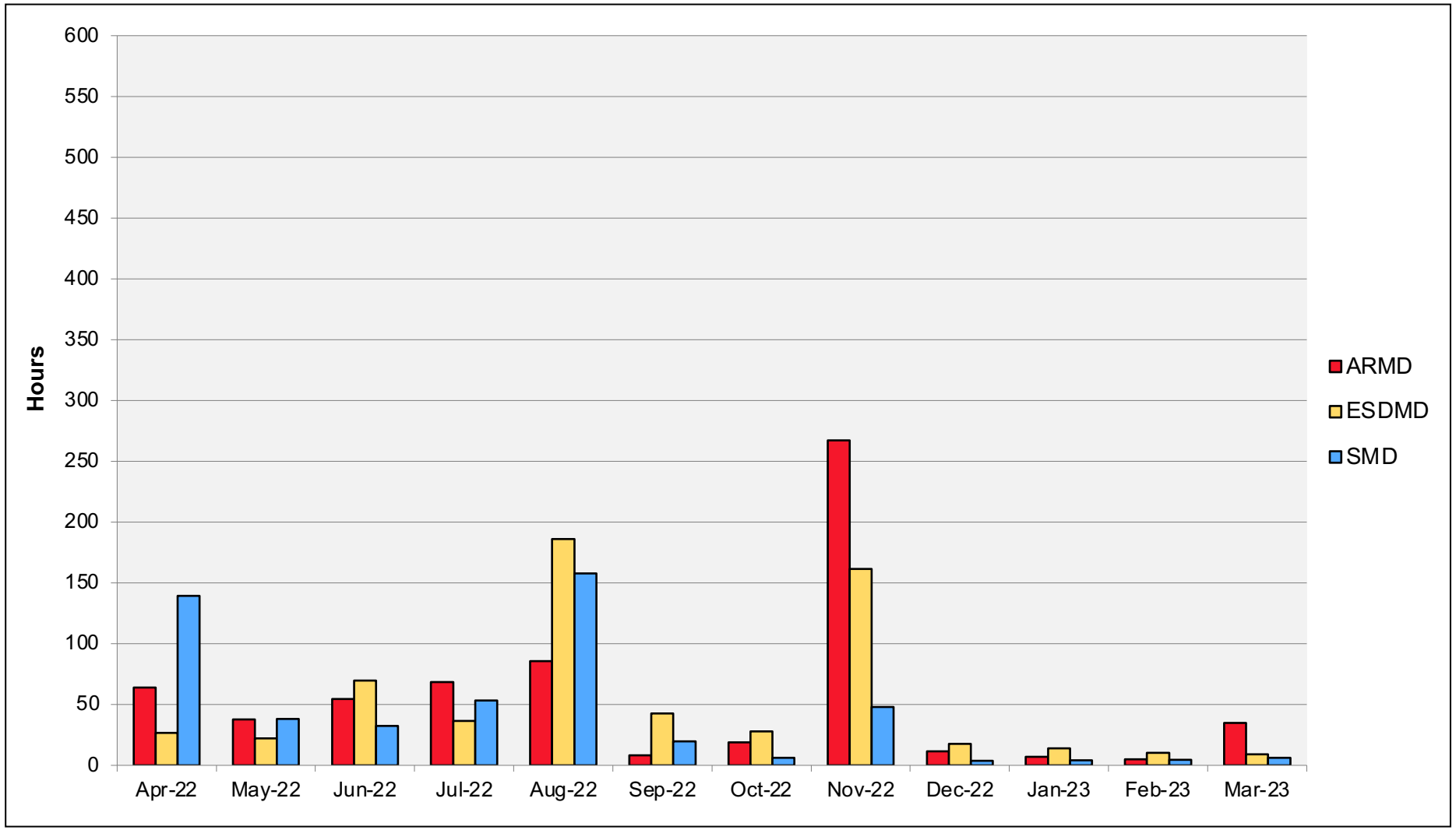
Aitken: Monthly Utilization by Job Size



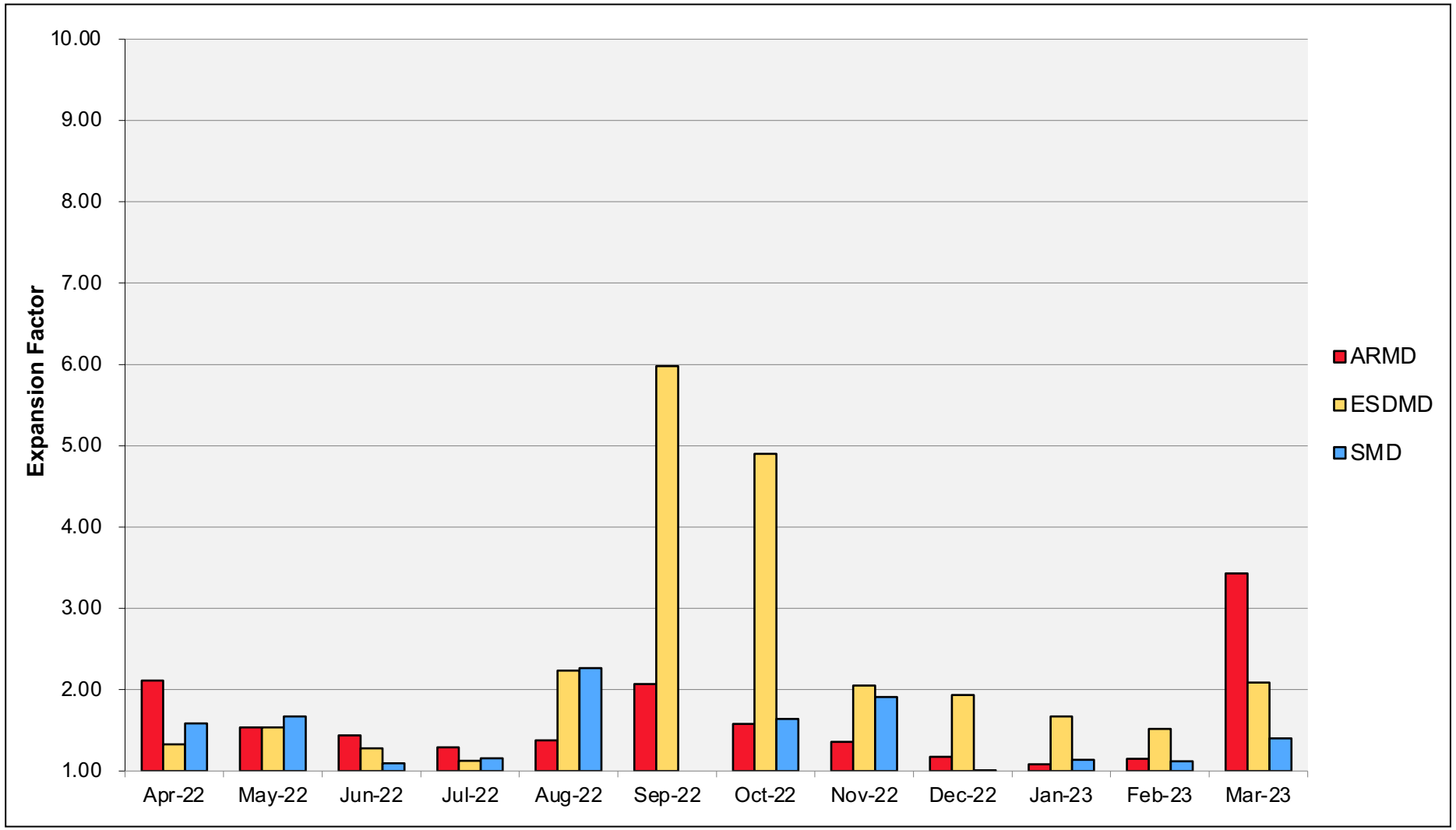
Aitken: Monthly Utilization by Size and Length



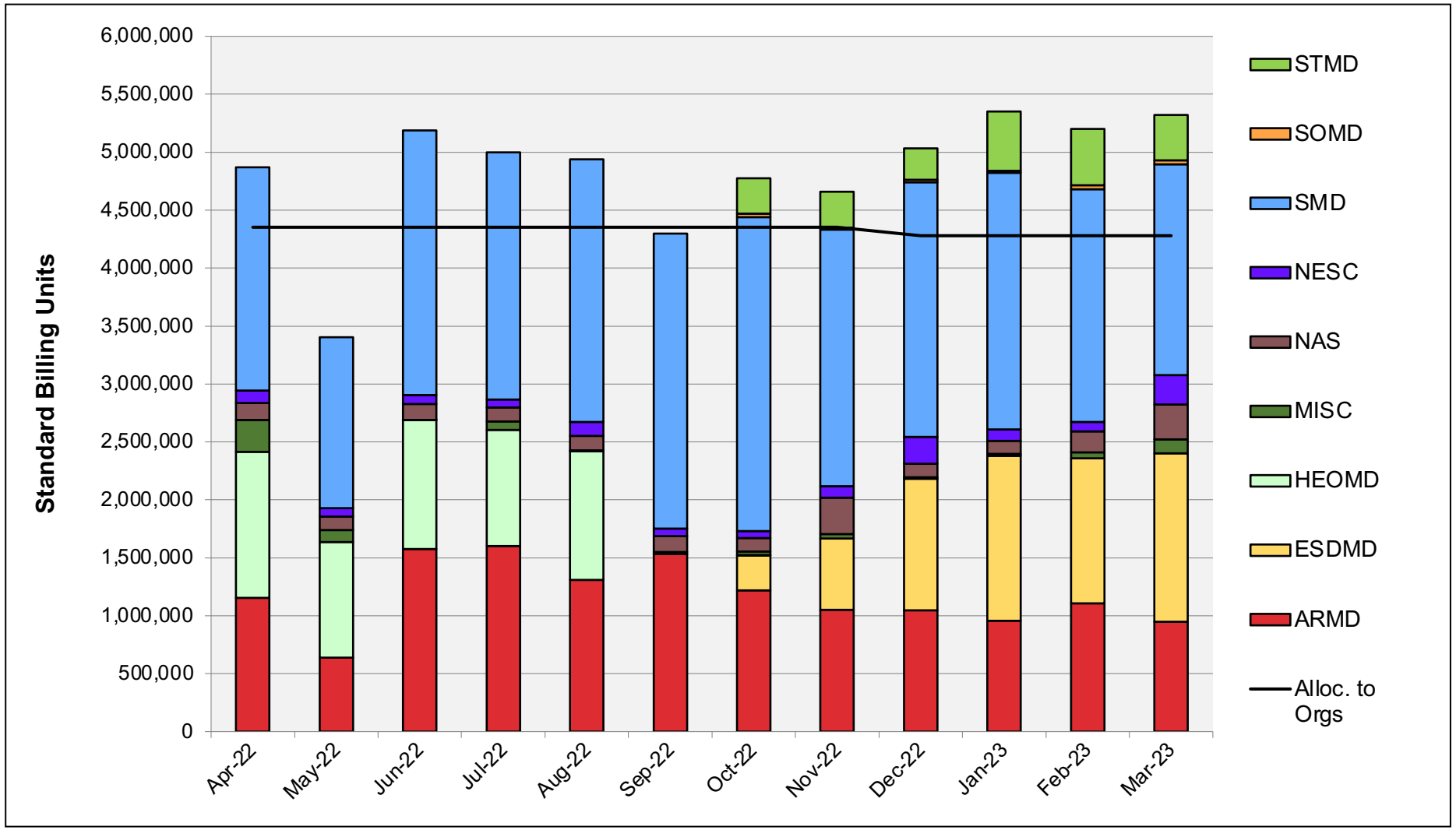
Aitken: Average Time to Clear All Jobs



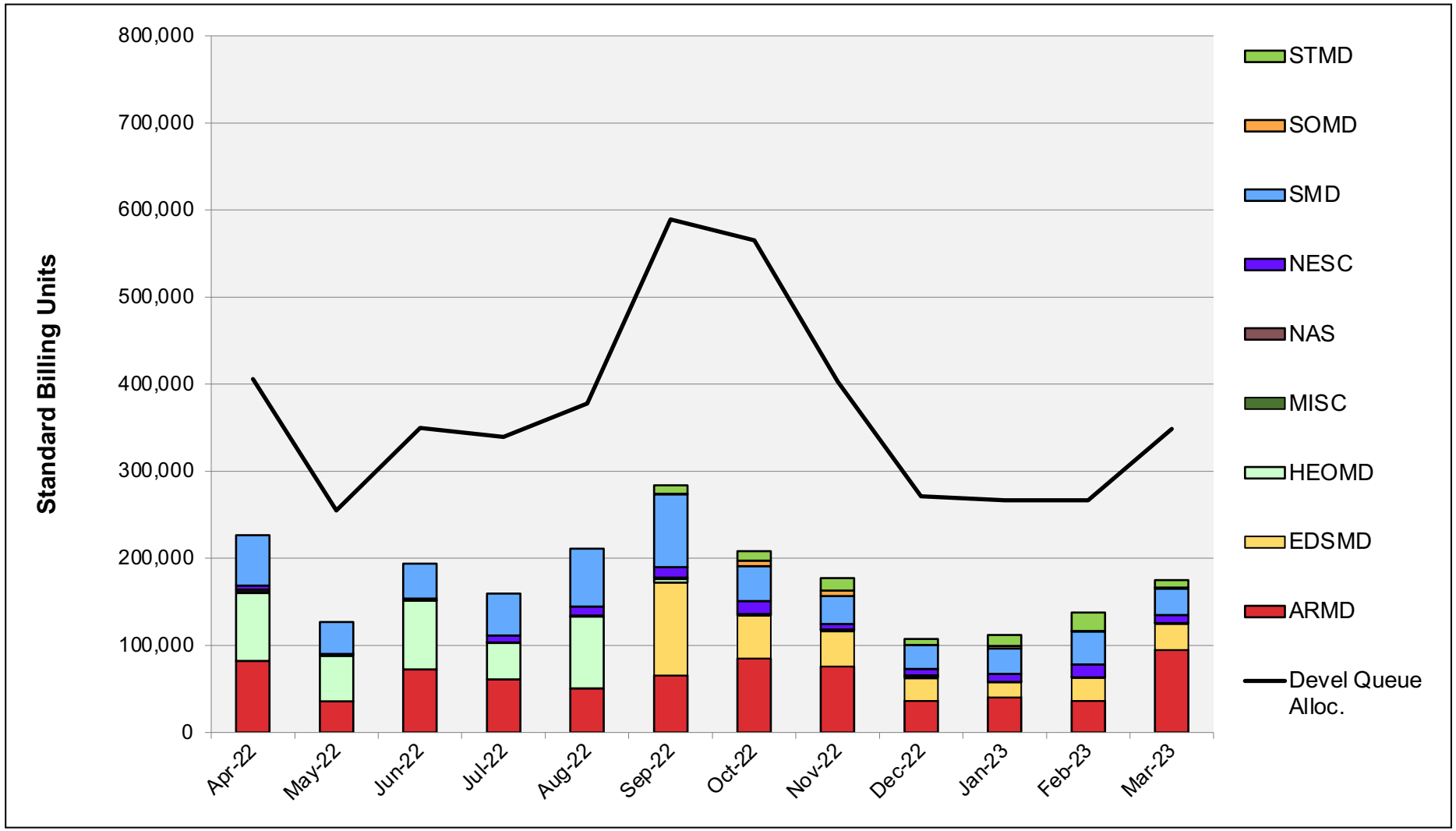
Aitken: Average Expansion Factor



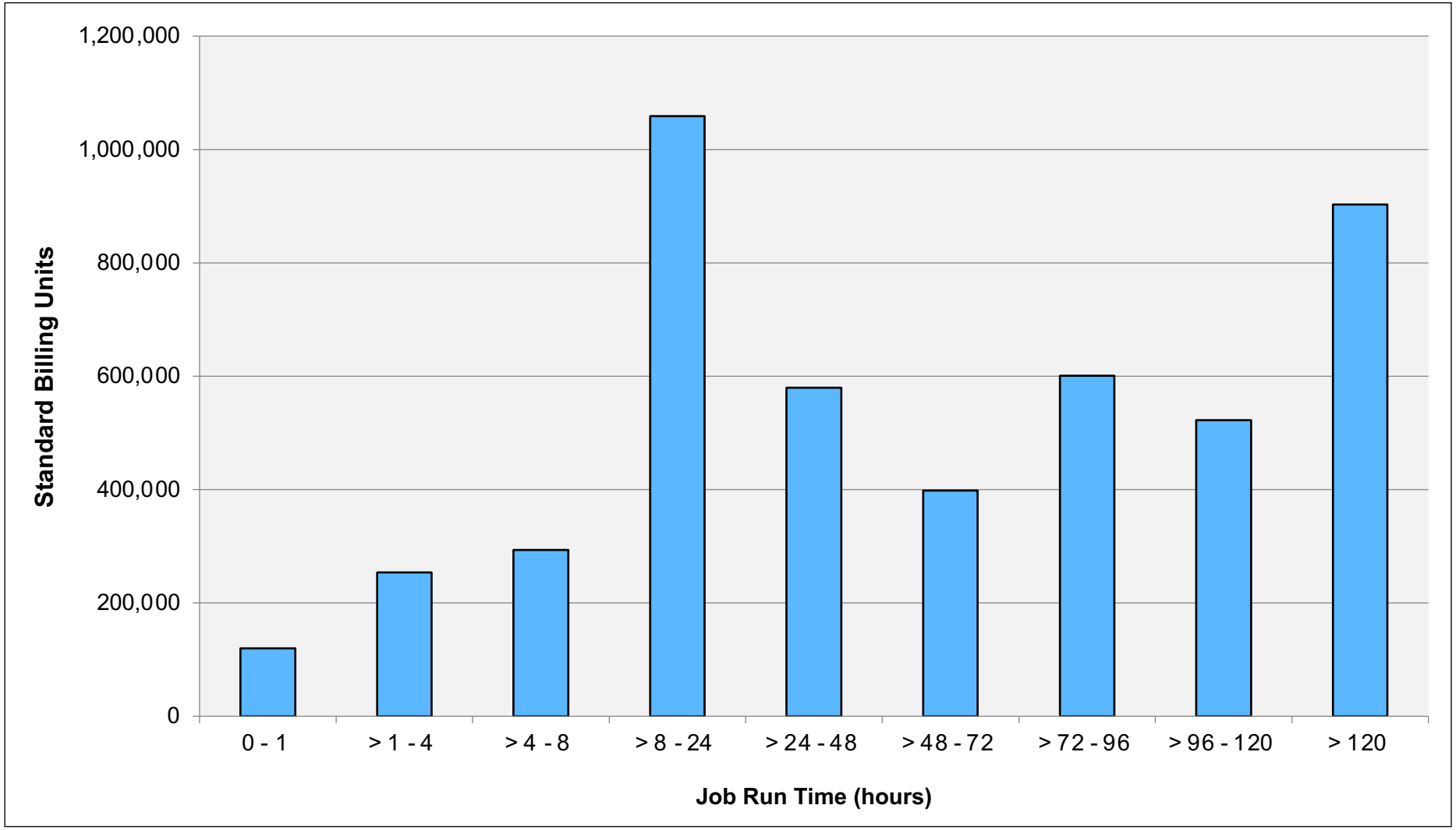
Pleiades: SBUs Reported, Normalized to 30-Day Month



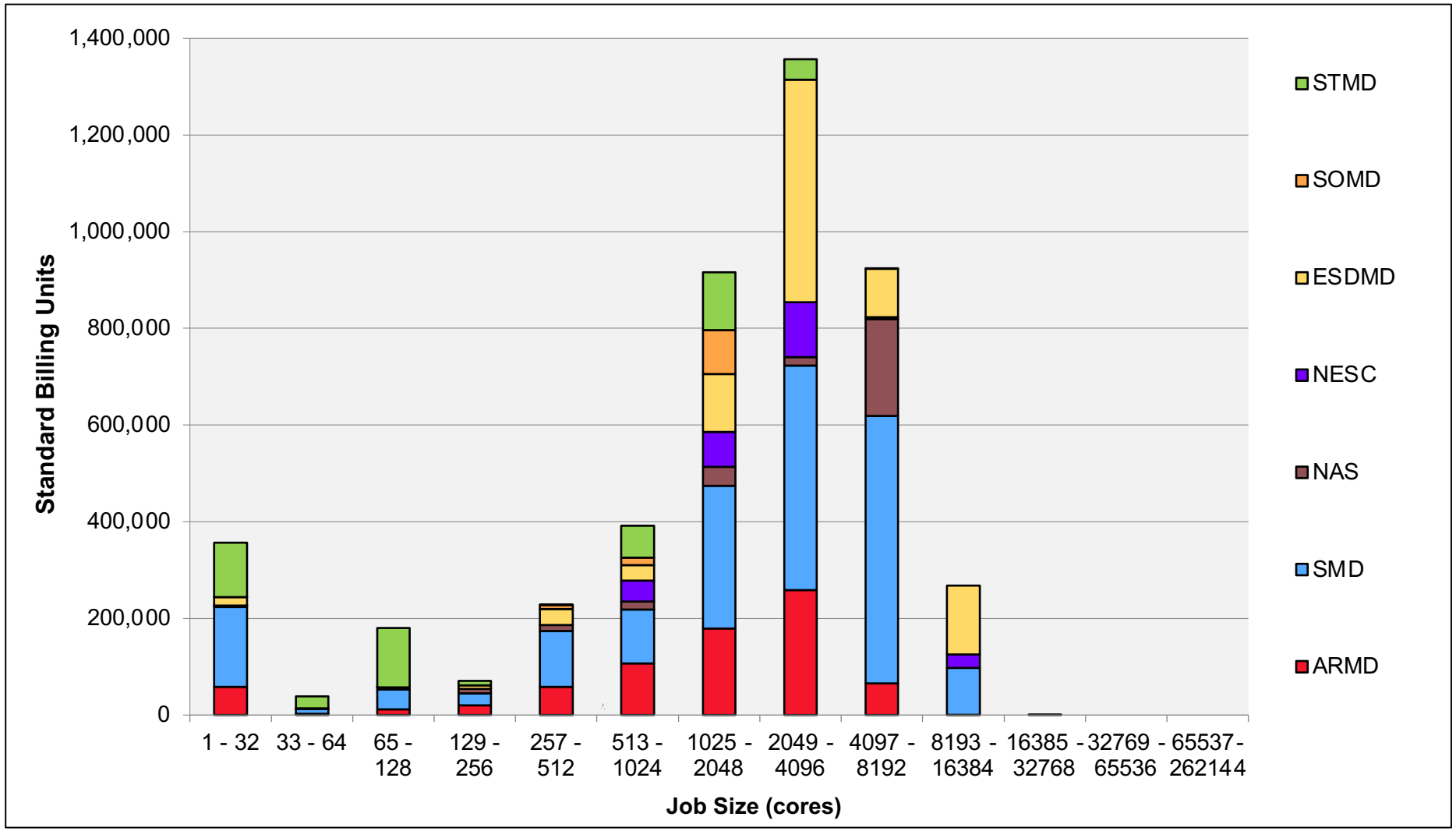
Pleiades: Devel Queue Utilization



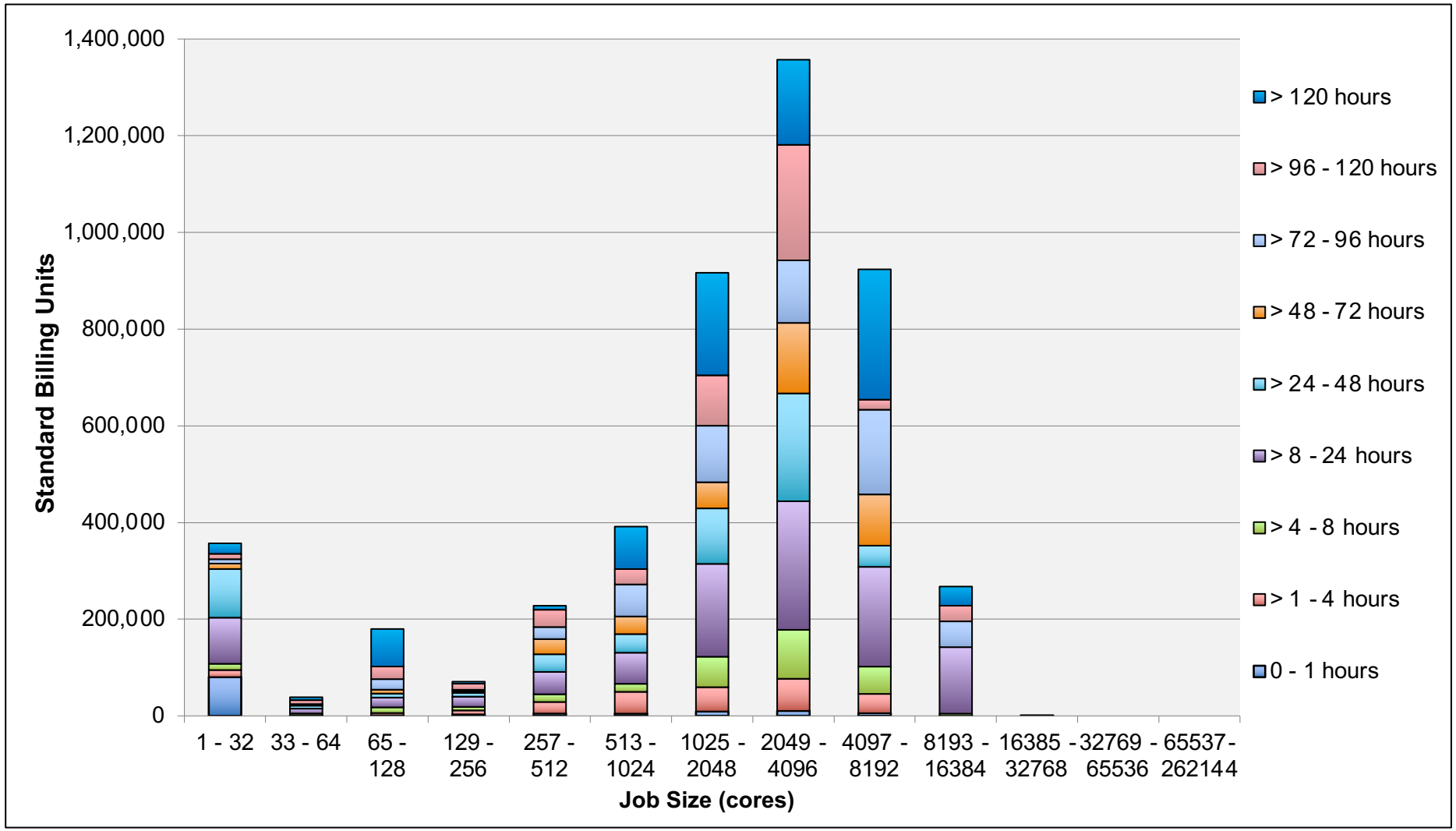
Pleiades: Monthly Utilization by Job Length



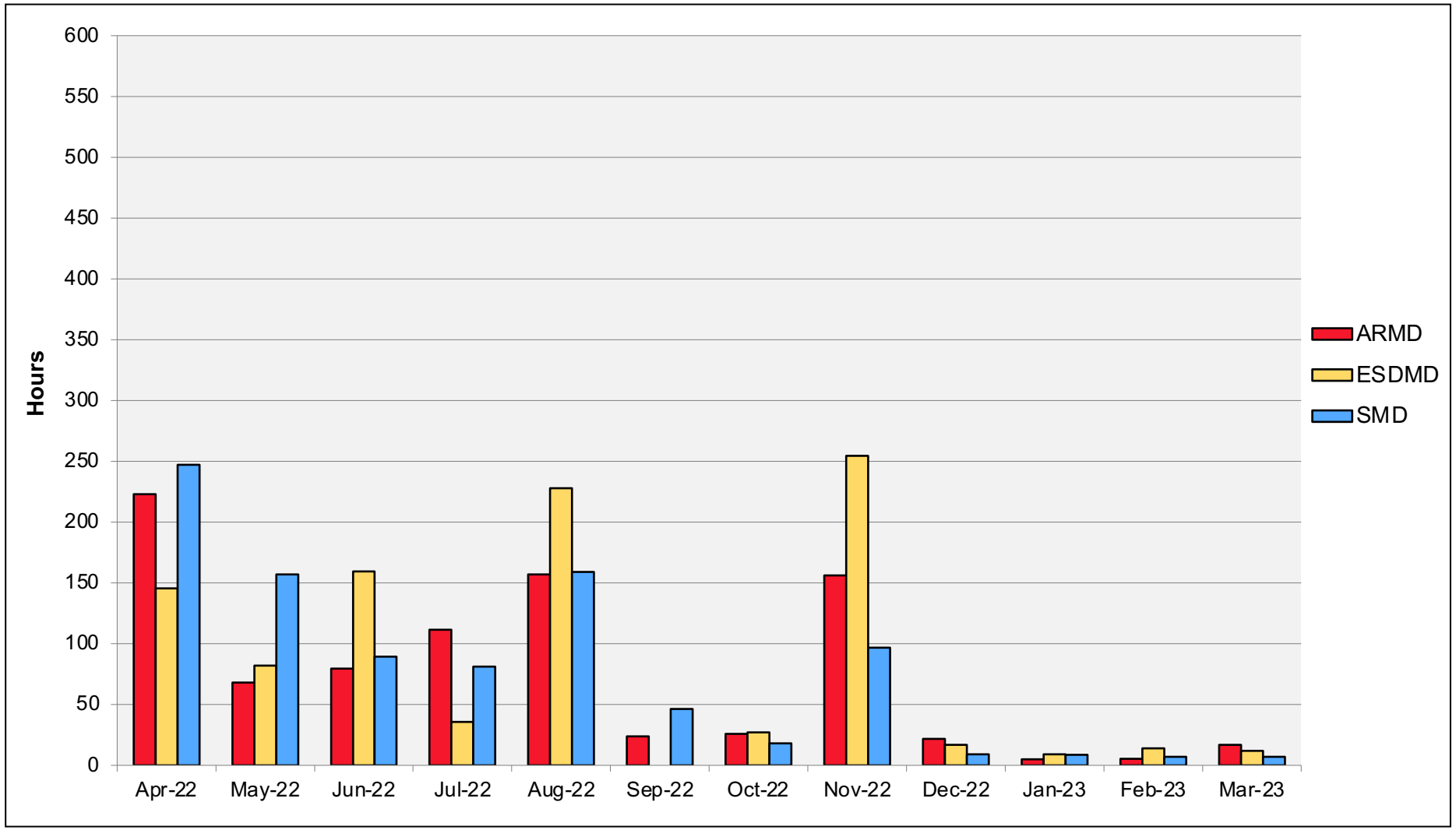
Pleiades: Monthly Utilization by Job Size



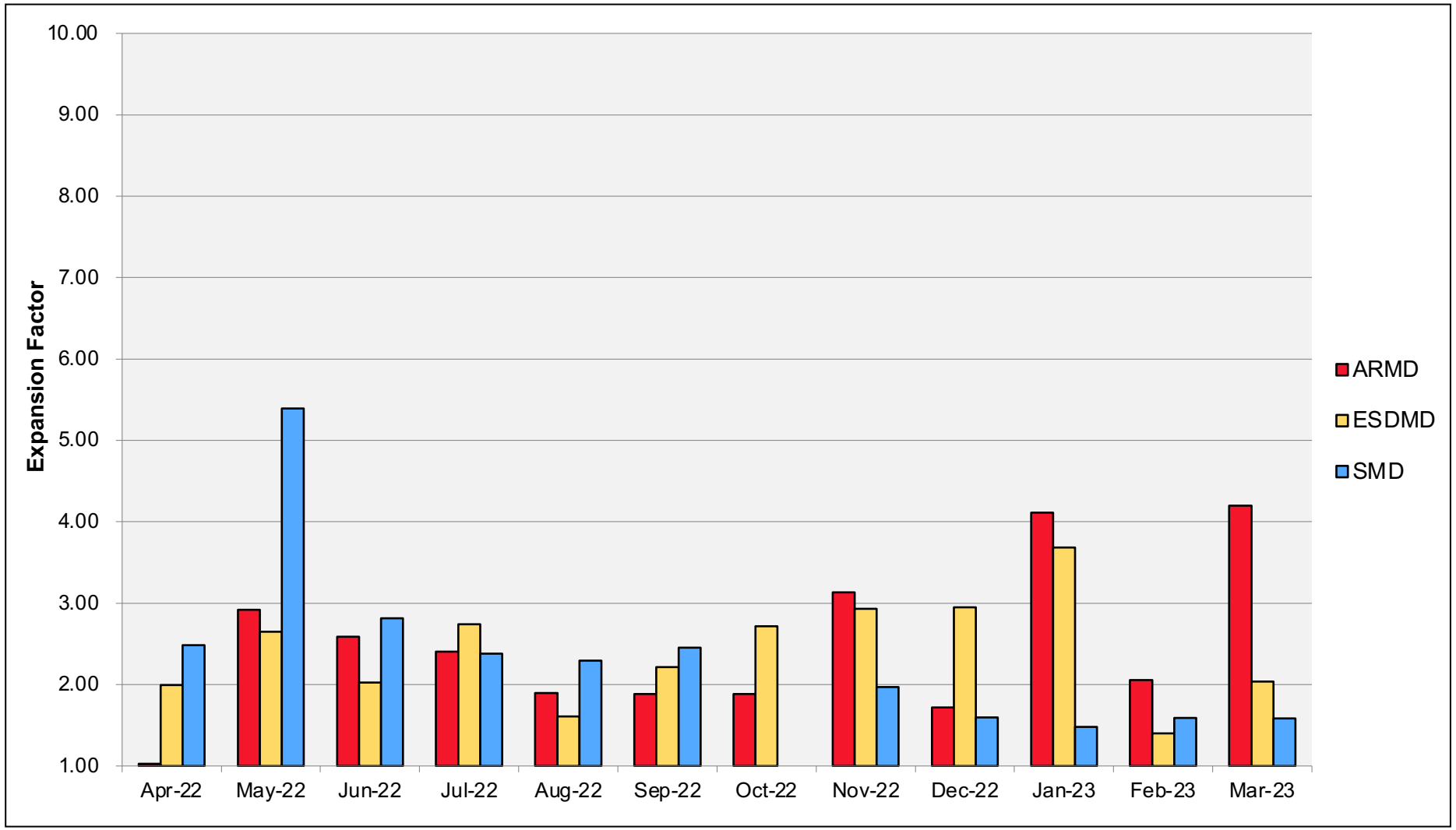
Pleiades: Monthly Utilization by Size and Length



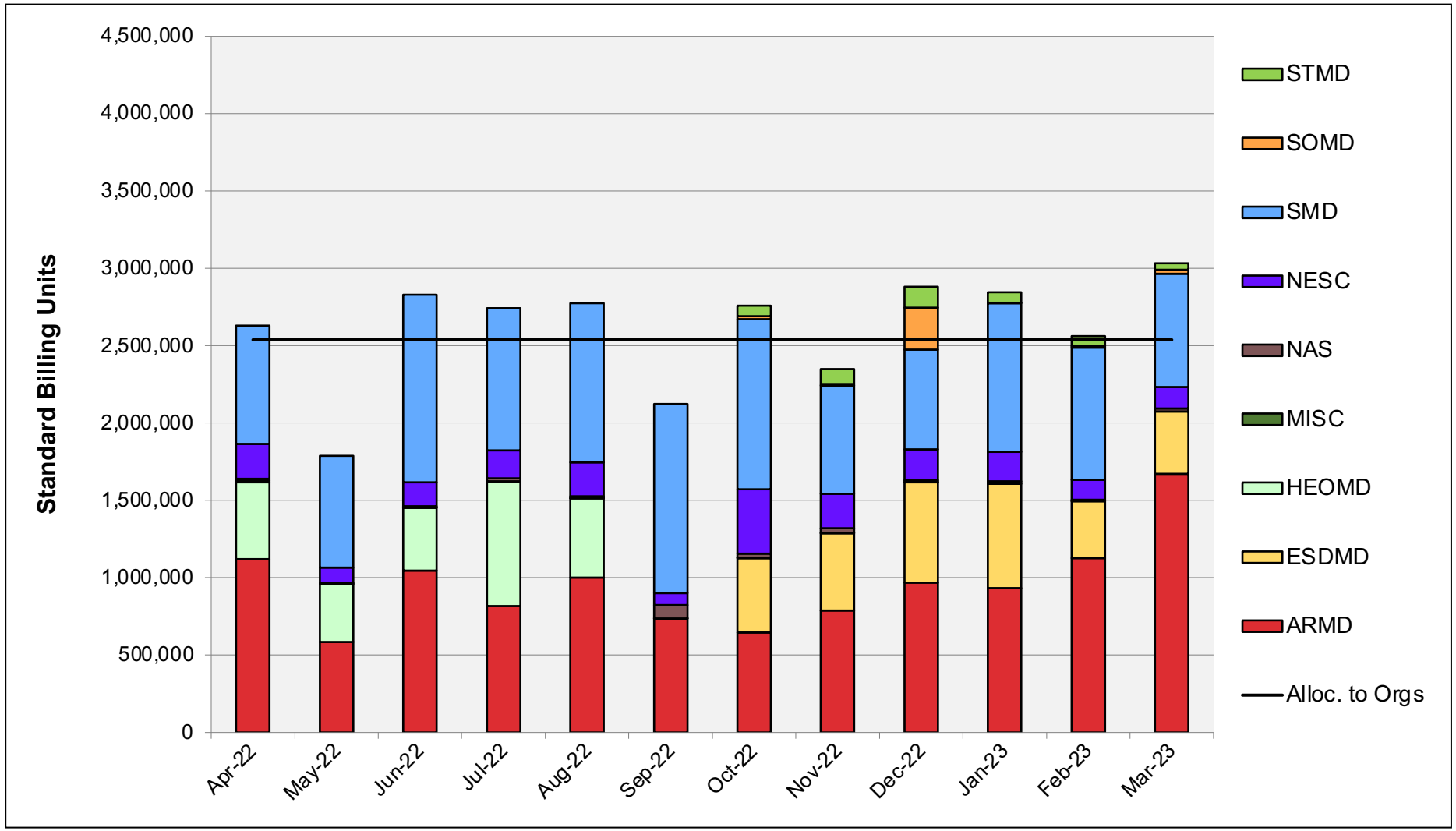
Pleiades: Average Time to Clear All Jobs



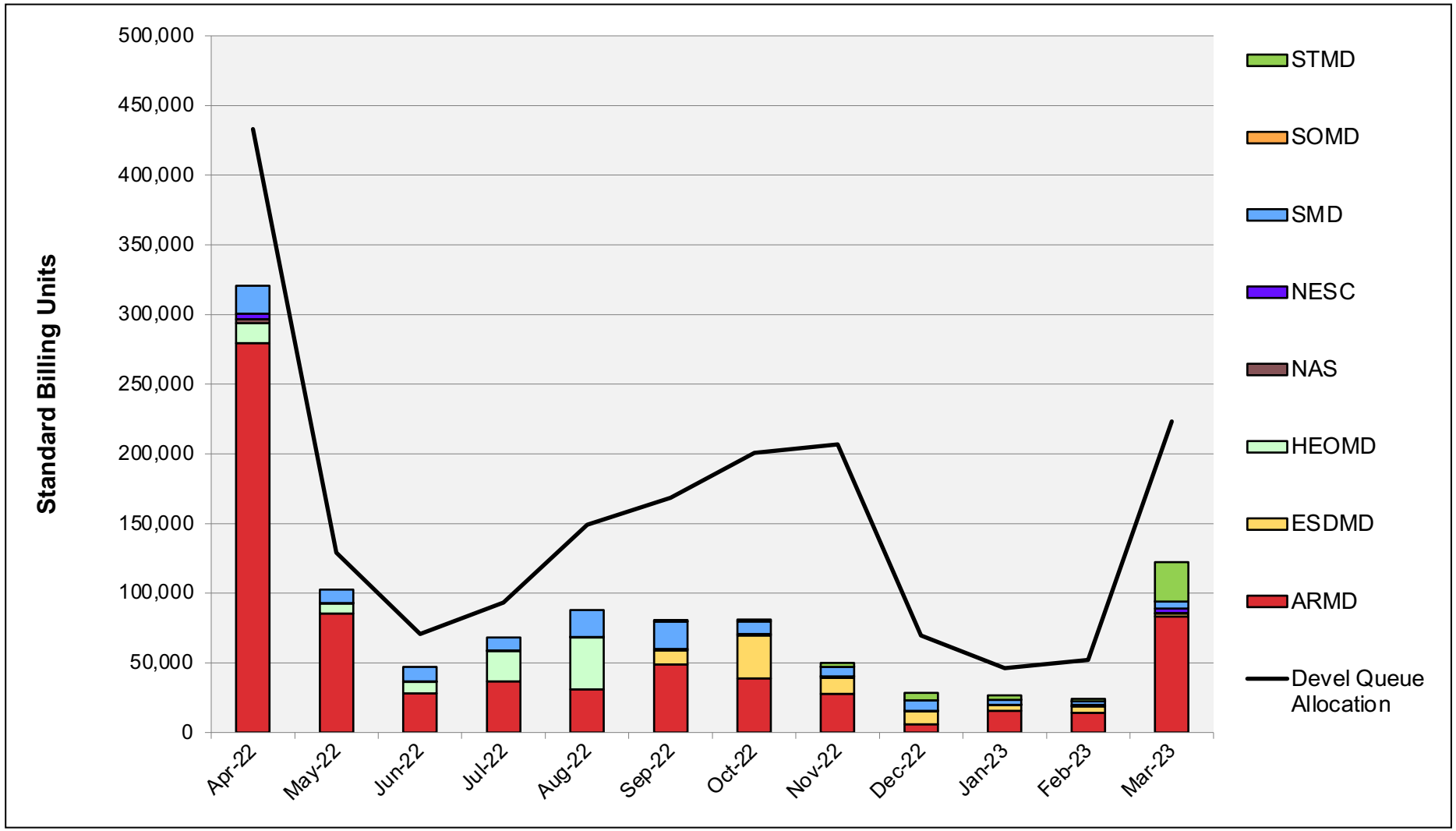
Pleiades: Average Expansion Factor



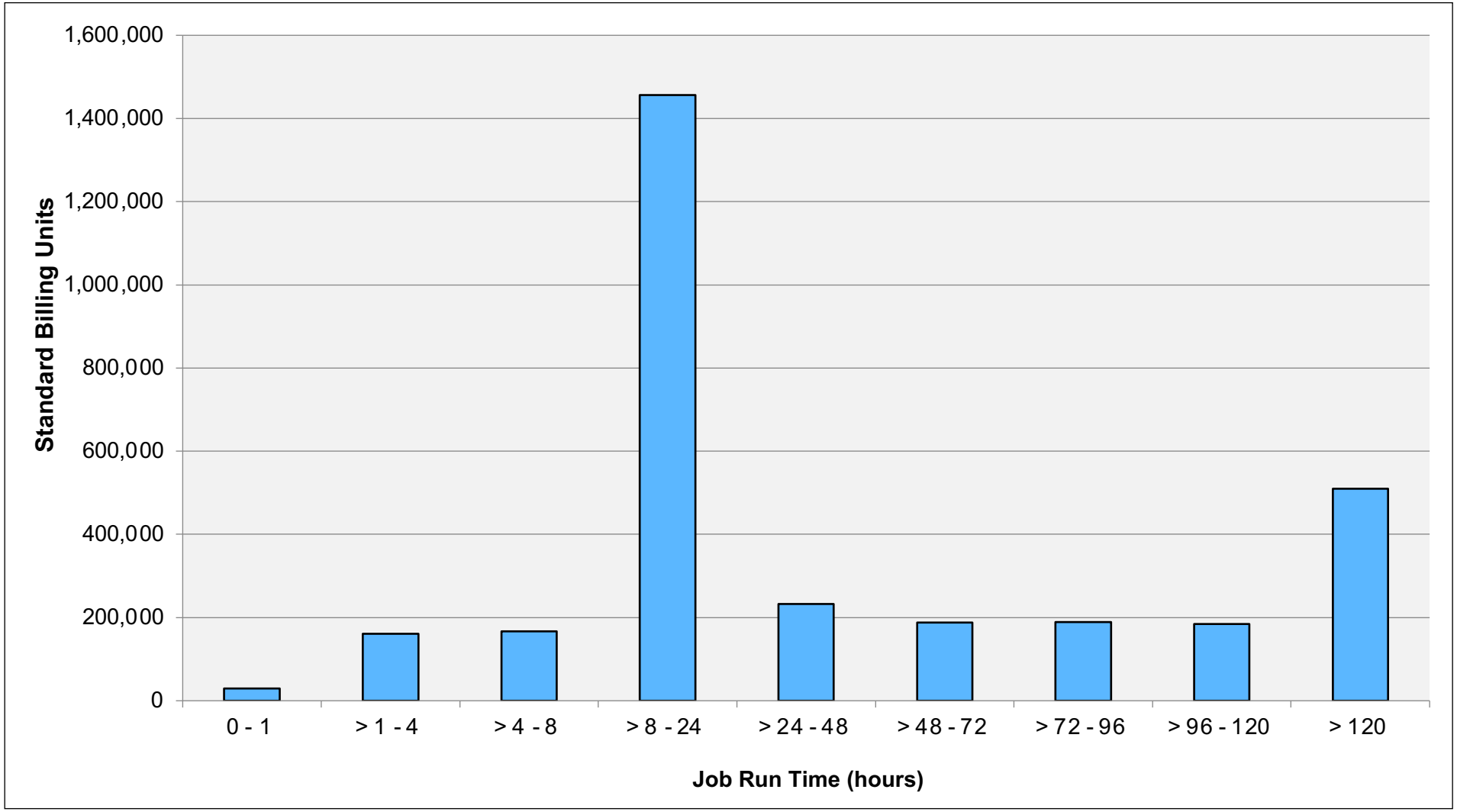
Electra: SBUs Reported, Normalized to 30-Day Month



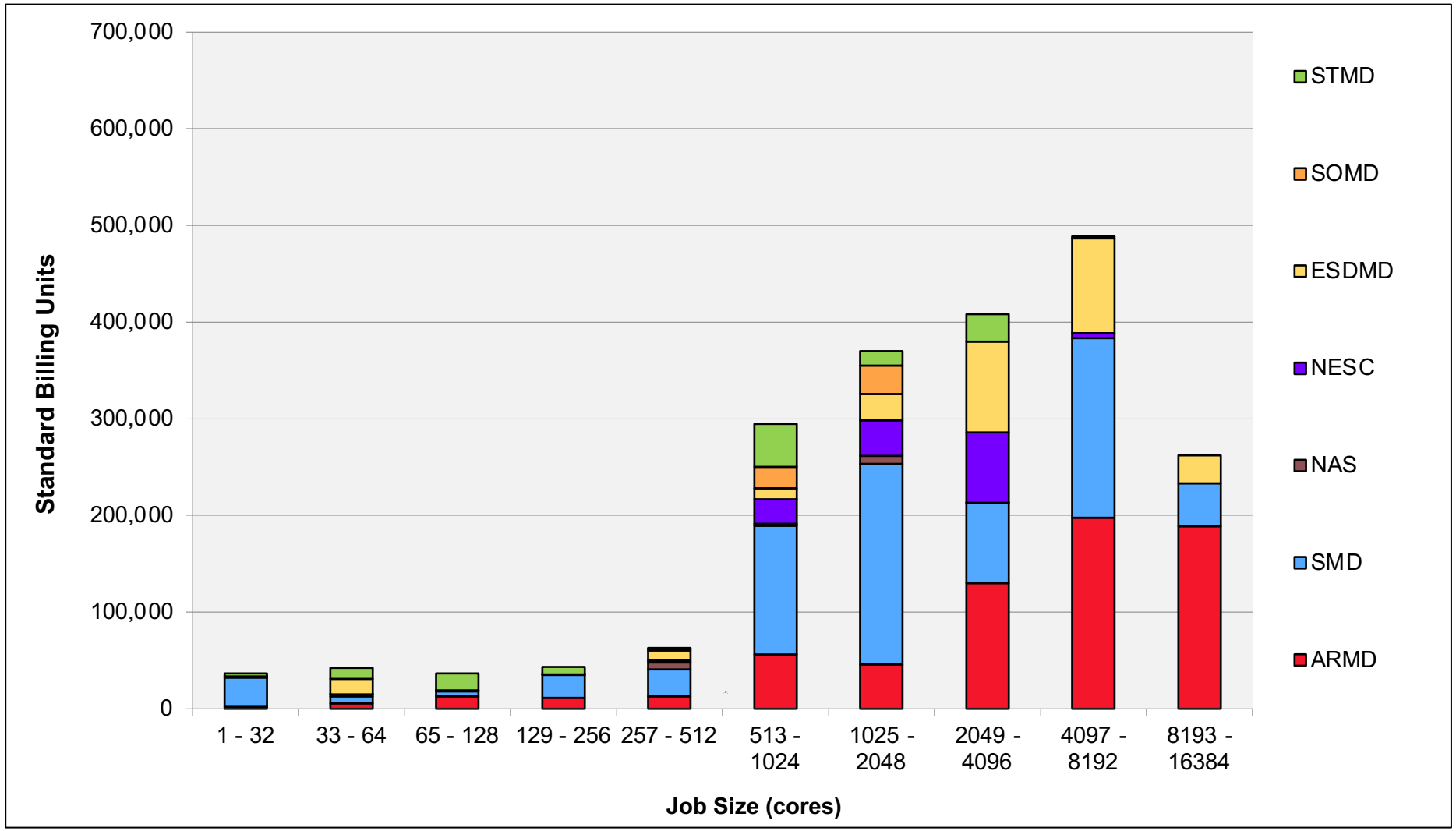
Electra: Devel Queue Utilization



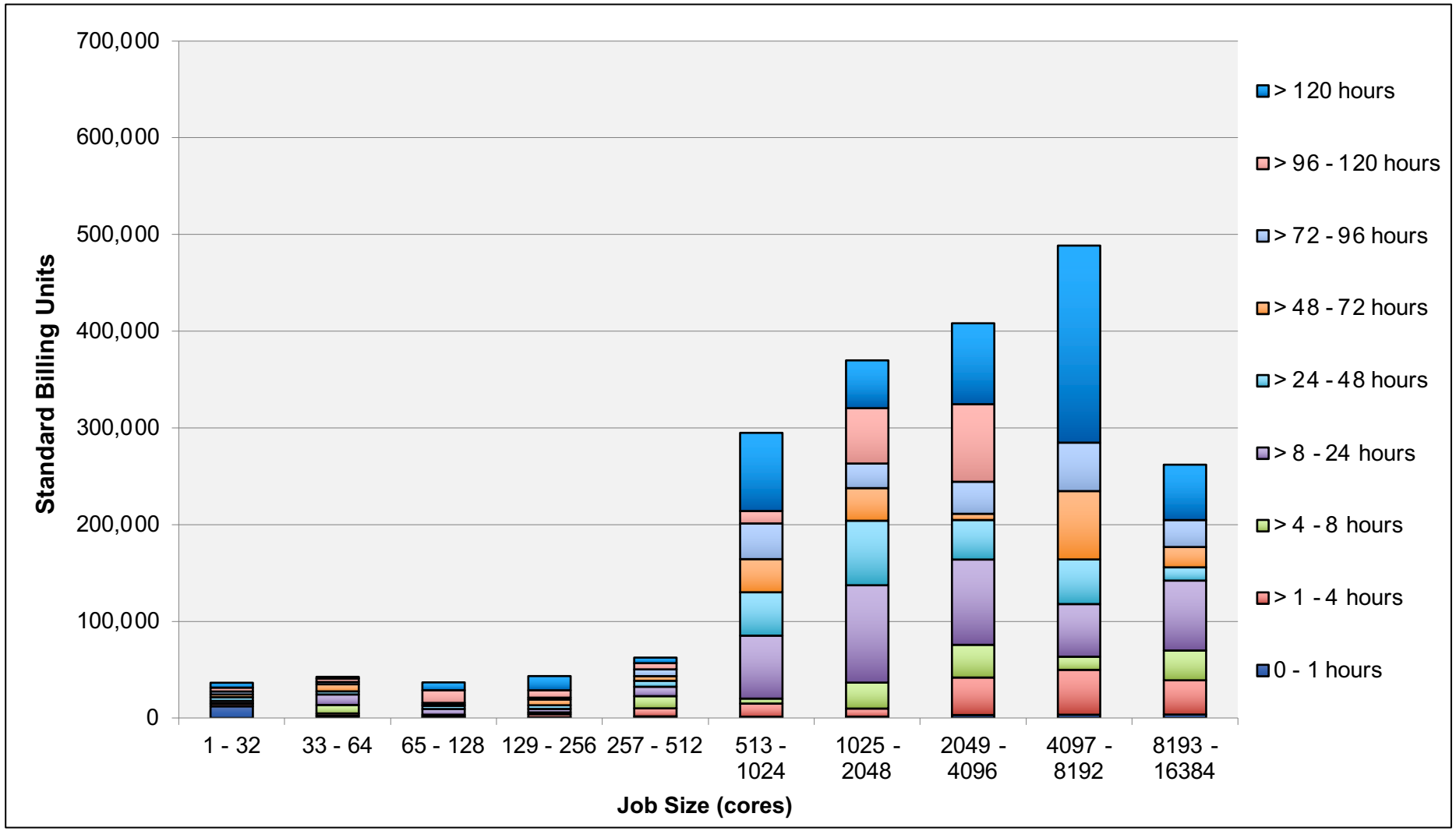
Electra: Monthly Utilization by Job Length



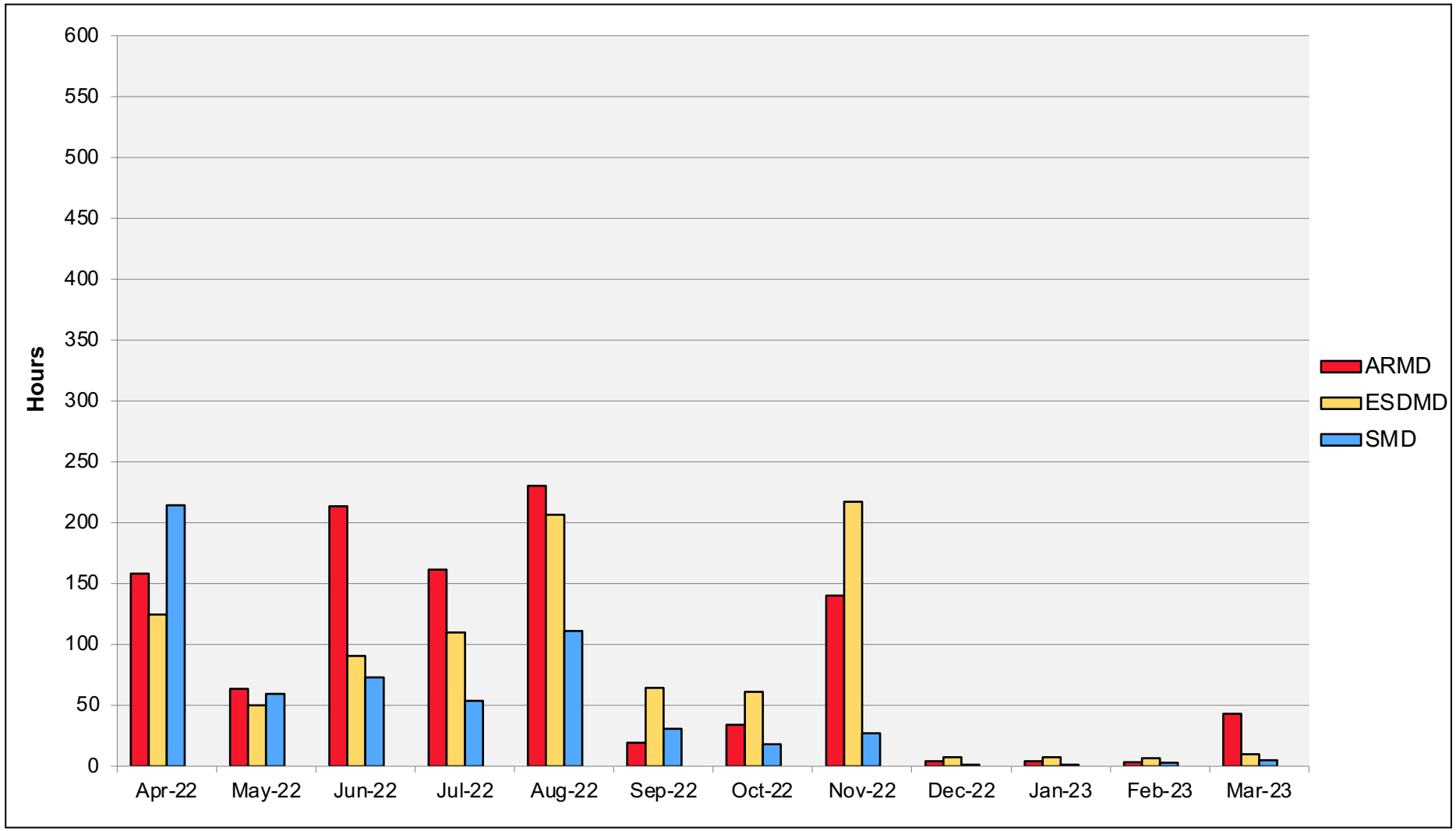
Electra: Monthly Utilization by Job Size



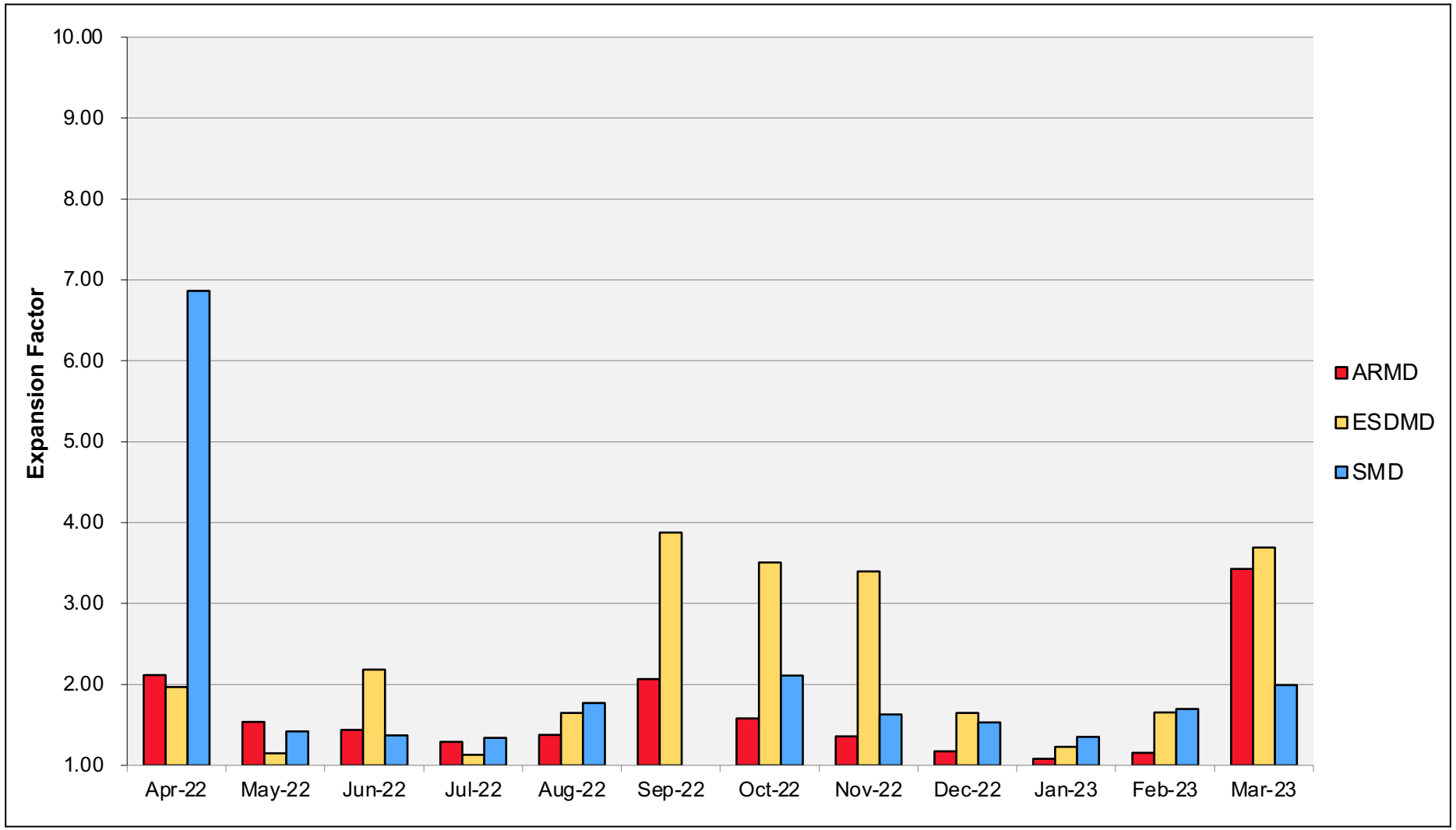
Electra: Monthly Utilization by Size and Length



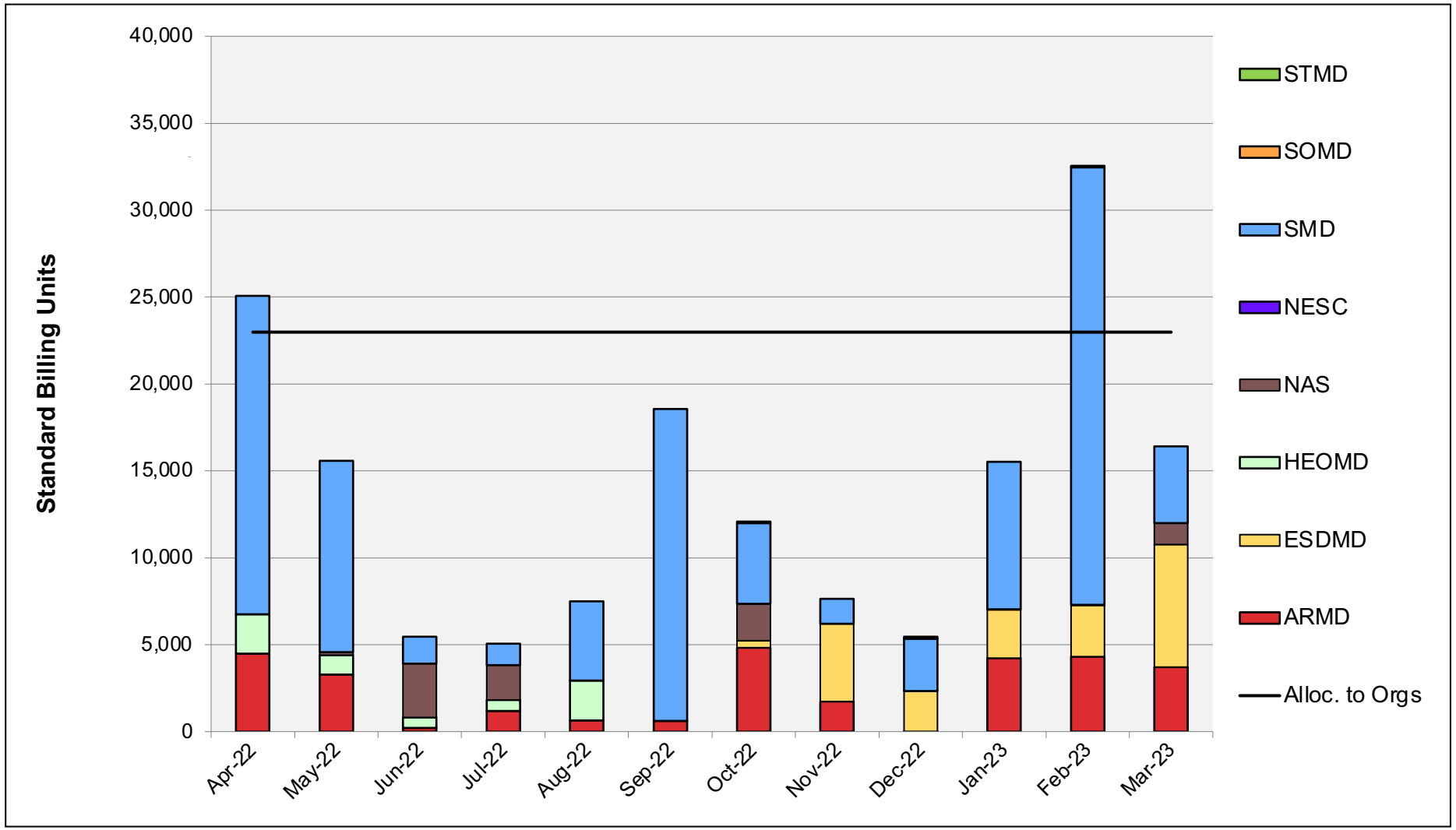
Electra: Average Time to Clear All Jobs



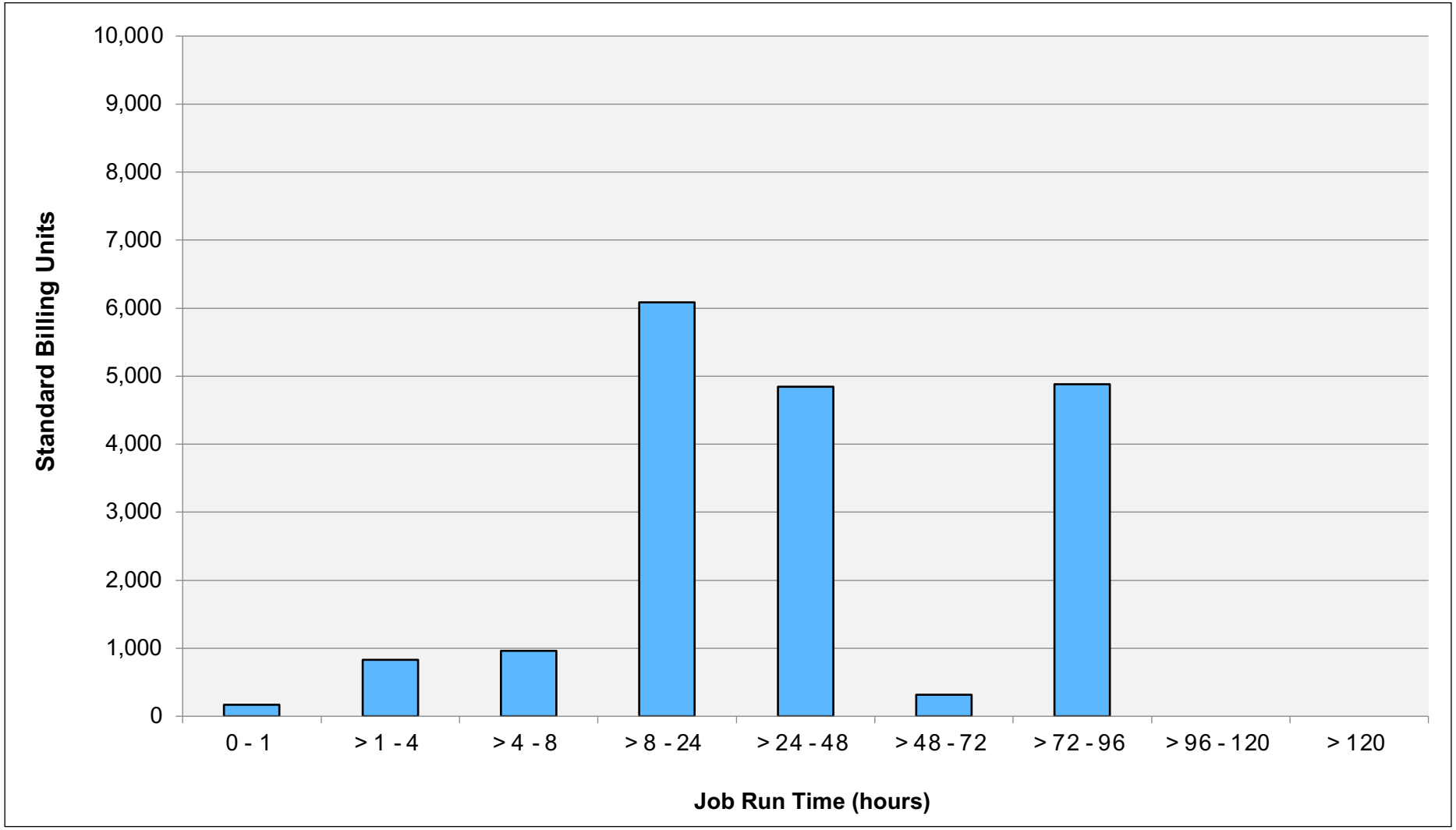
Electra: Average Expansion Factor



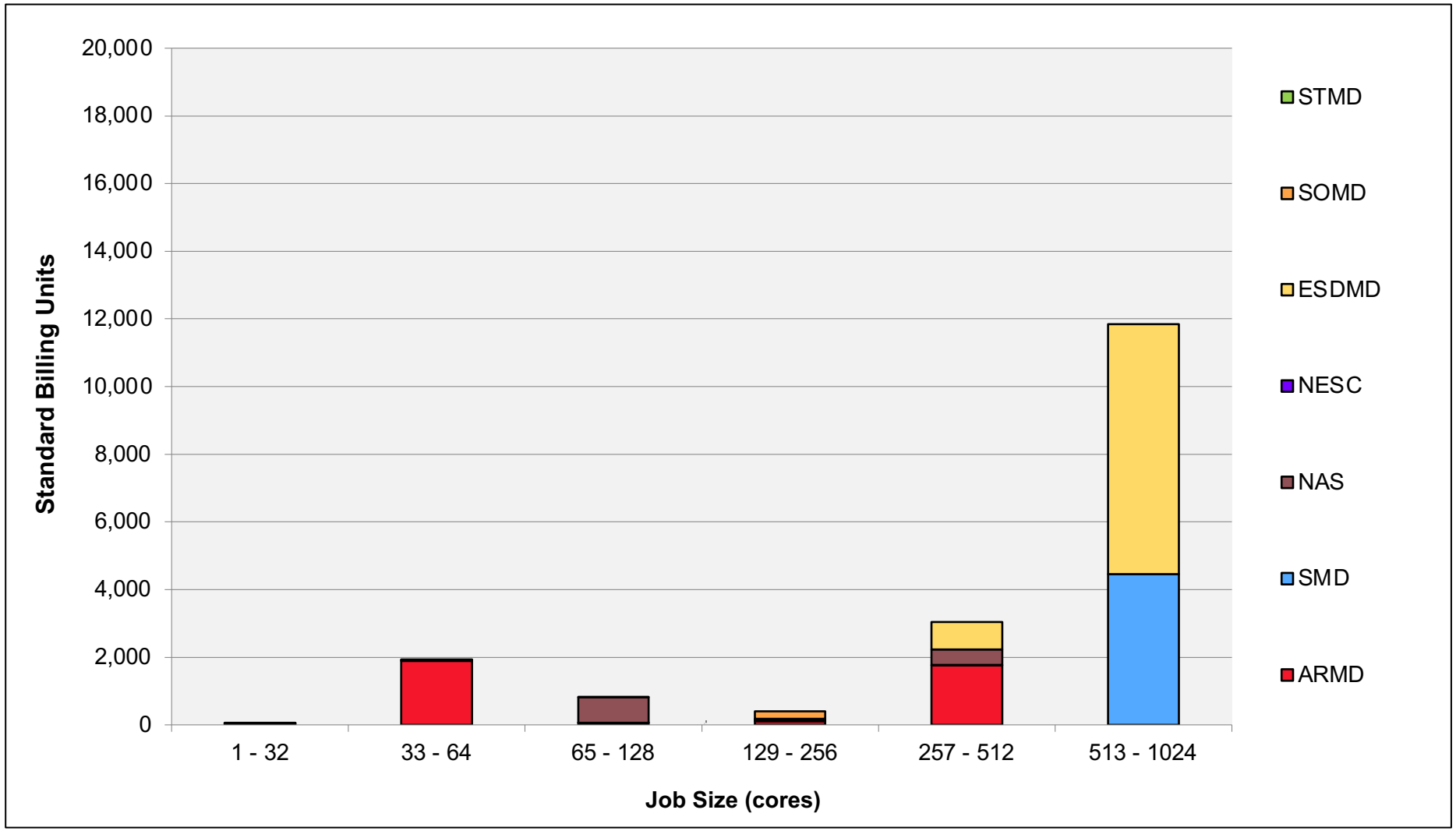
Endeavour: SBUs Reported, Normalized to 30-Day Month



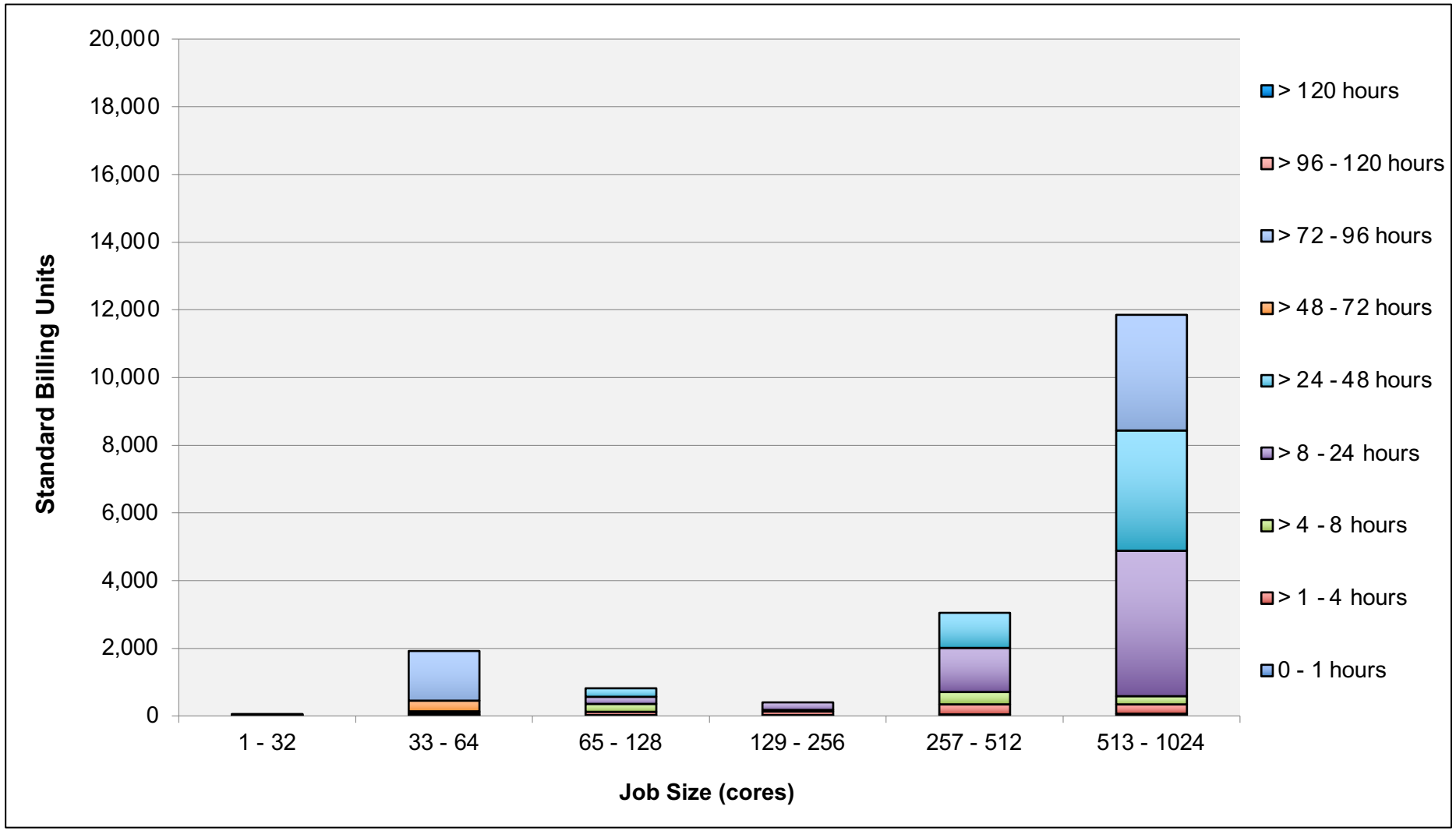
Endeavour: Monthly Utilization by Job Length



Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Expansion Factor